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**POSITIONS AND INTENSITIES S IN THE
 $3\nu_2/\nu_2 + \nu_4$ VIE! RATIONAL SYSTEM OF $^{14}\text{NH}_3$ NEAR 4 pm**

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Abstract

We report experimental line positions and intensities of the $3\nu_2$ and $\nu_2 + \nu_4$ bands of $^{14}\text{NH}_3$ obtained from 0.011cm^{-1} unapodized resolution spectra recorded with the Fourier transform spectrometer at Kitt Peak National Observatory.

1366 lines with $J' \leq 13$ have been assigned from which 1213 line positions with ($J' \leq 12$) are fitted using an effective rotation-inversion Hamiltonian to achieve a rms of 0.0069 cm-l . 726 intensity measurements are modelled to 12 terms of dipole moment expansion to $\pm 6\%$. The band strengths of $3\nu_2$ (s-a) at 2384.15 cm^{-1} , of $3\nu_2$ (a-s) at 2895.52 cm-l , of $\nu_2 + \nu_4$ (s-s) at 2540.53 cm-l , and of $\nu_2 + \nu_4$ (a-a) at 2586.13 cm^{-1} are estimated to be $0.61(3)$, $0.244(7)$, $0.186(3)$ and $0.174(25)\text{ cm}^{-2}\text{atm}^{-1}$ respectively, at 296 K .

A prediction of the line positions and intensities has been generated for all lines with intensities greater than $0.1,10^{-6}\text{ cm}^{-2}\text{atm}^{-1}$ at 296 K and submitted to HITRAN data base.

Beside the lines belonging to the $3\nu_2 / \nu_2 + \nu_4$ system a number of strong features appear in the spectra which could be assigned by a preliminary study to the hot bands ($\nu_3 - \nu_2$), ($\nu_1 - \nu_2$), ($4\nu_2 - \nu_2$).

Implications about the suitability of the Hamiltonian used is explored, given that the experimental accuracy is a factor of about 16 times better that has been achieved by the fit.

1. INTRODUCTION

Ammonia is the fourth most abundant constituent in the atmospheres of Jupiter and Saturn (1), after hydrogen, helium and methane. This relative abundance is attested by the presence in the infrared planetary spectra of many absorption features observed not only in the range of fundamental bands but also of higher overtone/combination bands. For example in the 4pm range, which is of special interest for probing deep atmosphere layers in both planets, the observed ammonia absorption arises primarily from the $3\nu_2/\nu_2 + V_4$ system of $^{14}\text{NH}_3$. In order to interpret current high quality planetary spectra (2,3) it is necessary to have a complete and accurate prediction of the ammonia contribution before any new planetary constituents can be identified in this region.

While the 4 μm band system of $^{15}\text{NH}_3$ species was studied in the recent past (4), the $3\nu_2/\nu_2 + v4$ system of $^{14}\text{NH}_3$ was so little investigated (5,6) that planetary analyses were forced to rely on the assignments and band strengths reported by Benedict et al (5) in 1958. Our purpose in the present work is to obtain the required spectroscopic data of this vibrational system for the main isotope with the same level of accuracy as those obtained in the recent past for other important absorbers in the range, namely $^{12}\text{CH}_4$ (7-9), $^{13}\text{CH}_4$ (1 O) and PH_3 (11,12).

Due to the large inversion splitting of the ν_2 vibrational mode, the $3\nu_2/\nu_2 + \nu_4$ system covers an extended range, as seen in Fig. 1. The two overtone components $3\nu_2(s \leftarrow a)$ and $3\nu_2(a \leftarrow s)$, centered at 2384.15 and 2895.52 cm^{-1} respectively, are no less than 511.37 cm^{-1} apart. The two combination band components $V_2 + V_4(s \leftarrow s)$ and $V_2 + V_4(a \leftarrow a)$ are located midway at 2540.53 and 2586.13 cm^{-1} respectively. Accordingly, the present study used 0.011 cm^{-1} (unanodized) resolution spectra of NH₃ recorded in all the range of 1800 to 5400 cm^{-1} with the McMath Fourier transform spectrometer located at Kitt Peak National Observatory; these data were part of a larger set obtained for analysis of the 2 pm region (by the third author). An example of the 4 pm region is shown in Fig.2. Because of the weakness of the $V_2 + V_4$ band relative to the $3\nu_2$ band, several optical paths were required.

Line assignments were carried out as thoroughly as possible up to $J' = 12$ in the four vibrational components. Line positions and intensities were analyzed within a dyad system in order to account properly for the Coriolis-type interactions between the $3\nu_2$ and $V_2 + V_4$ bands. Finally, the energy and intensity parameters derived from the analyses were used to generate a line-by-line prediction of the spectrum suitable for planetary applications. Although not included in the present article, the spectral data contained many transitions of hot bands. Measurements of these unassigned features were tabulated and combined with the dyad prediction for the 1995 editions of the HITRAN (13) and GEISA databases (14).

II. Experimental, DETAILS

Laboratory spectra of ammonia were recorded at 0.011 cm^{-1} unapodized resolution using the Fourier transform spectrometer located at the McMath telescope at Kitt Peak National Observatory. The infrared signal from a globar source was selected for the 1800 to 5500 cm^{-1} band pass and detected by InSb detectors. I-he sample chambers were a 1.5 m stainless steel single pass cell and a 6 meter base multiple-pass chamber. Gas pressures were monitored continually with capacitance manometers during the one hour period used to record each spectrum. Gas conditions of the six spectra used for the present study are shown in Table 1. For several spectra, a second absorption cell containing CO was placed in the path to provide calibration of the line centers. The data usually contained residual absorption from H_2O and CO_2 arising in the purged air path between the source, cell and FTS. However, this background contamination was substantially reduced with respect to previous works (5).

Line intensities and most line positions were retrieved from these data through curve-fitting of the unanodized and uninterpolated spectral digits. For this, differences between the observed and synthetic spectra were minimized by iterating the position, intensity and width of each spectral feature (15). Some line positions from the most dense scans were obtained by peak-finding of the apodized and interpolated spectrum. The measured line centers of CO were compared to those tabulated by Maki and Wells (16) to establish a multiplying factor to apply to all the retrieved line positions. The agreement with the calibrated CO positions was 0.00003 cm^{-1} . Table II gives a sample of the resulting individual measurements for a few lines showing the averaged and individual measurements of positions and intensities obtained from runs 1, 2, 3 and 5. From these comparisons, it appears that the retrieval precision might be 0.0001 cm^{-1} or better for positions. However, the precision for positions is degraded by self-broadening pressure shifts, and there is not sufficient information available to make precise corrections. A recent study of V_2 transitions near 900 cm^{-1} (17) reports that shifts for 11 lines are both negative and positive and range from 0.66 to 3.77 MHz/Torr . If pressure shifts increase proportionally with frequency, then an approximate shift for NH_3 lines at $4\text{ }\mu\text{m}$ would vary from 2 to 11 MHz/Torr . In table II., there is some indication of shifts in that the 6.5 Torr data has either the lowest (or highest) observed positions of the four runs, but the largest difference is 0.00042 cm^{-1} . Thus with strong well-isolated lines for which at least three scans have been used, positions are thought to be accurate to 0.0002 cm^{-1} or better. This is also indicated by inspection of the combination differences.

The intensities were retrieved from four of the spectra. The remaining run (#4) was not measured for intensities because the sample pressure dropped 12% during the one hour integration, During the data reduction, it was found that the intensities from run #2 differed by a constant amount from those taken from the short path cell, and the measurements were

normalized to agree with scan #1 so that effectively the intensities are based on three independent optical densities. Individual retrieved intensities were averaged together only if the features had absorption depths between 6 and 80%. The precision of well-isolated lines are $\pm 2\%$, but because of the behavior of the NH₃ gas sample, the absolute accuracy of the intensities is set conservatively to $\pm 5\%$ for these data.

The quoted accuracies for positions and intensities apply only to the well-isolated transitions. A comparison of spectra showed that only 35 to 55% of the total available features are clean features depending on the spectra. All other lines are blended transitions or weak features measured on the shoulders of stronger saturated lines.

III. THEORETICAL MODEL

Our present vibration-rotational approach of the 3v₂/v₂ + v₄ system is formally quite similar to that previously developed to investigate other interacting systems in C_{3v} molecules (11, 12, 18, 19). All the couplings between 3v₂/v₂ + v₄ and outer interacting bands were assumed to be weak enough to be taken into account properly by a perturbation treatment via Contact Transformation method. The limitations of this approach which will be detailed in section V, can be inferred from fig. 1, which gives the position of the first vibration and inversion levels of NH₃. Accordingly rotational energy levels and line intensities were calculated using effective Hamiltonian and dipole moment operators built up suitably for the system under investigation.

In the case of usual semi-rigid C_{3v} molecules, like CH₃D (18, 19) and even PH₃ (11, 12), these operators were obtained as expansions in serial power of all normal coordinates and momenta. Presently for NH₃, such an expansion is not valid, due to the large amplitude motion associated with the V₂ inversion mode. The treatment of the vibration-inversion-rotation in NH₃ has suggested an important number of studies in the past. A parametrization of the energy levels that is very convenient for our present purpose was developed by V. Spirko et al (20), and later by S. Urban (21). Similar parametrization for the intensities was more recently introduced by S. Pracna et al (22).

In all those studies, the large amplitude inversion motion is removed from the vibrational problem and treated together with the rotation. The usual way to achieve this goal is to choose a reference configuration which follows the large amplitude motion in such a manner that all other vibrational motions remain small (23). This reference configuration is

usually chosen to be planar with the D_{3h} symmetry, according to the double minima potential function.

Fig. 3 illustrates schematically the structure of the upper state energy matrix with all the interacting blocks between $v_2=3$ and $V_2=v_4=1$. In Table III, the exact expression of these energy matrix elements is given. Table IV contains the transition dipole matrix elements corresponding to the transitions investigated in the $3v_2$ and $v_2 + v_4$ bands. The elements given in both tables are consistent with the phase conventions used in Ref. (24). The basis wavefunctions used in Table III and IV are the eigenfunctions of the zero order Hamiltonian, labelled $|i, V_2, V_4, I_4; JKM\rangle$ according to Ref. (20) where $i = s$ or a represents the inversion symmetric and antisymmetric components, respectively. As in Table III, the expansion of the terms shown in Table IV is limited to the order of magnitude required to achieve the present fits for line positions and line intensities given in section IV.

Three kinds of matrix elements are involved in the energy matrix at the order of magnitude used : a) diagonal matrix elements; b) diagonal matrix elements in the vibrational quantum numbers V_2 and V_4 but off-diagonal in all other quantum numbers K , I_4 and i ; c) Coriolis-type matrix elements coupling $V_2=3$ and $v_2=v_4=1$ states which are of two kinds, $\Delta K=\pm 1$, $\Delta I_4=\pm 1(s<\rightarrow>s)$ or $\Delta K=\pm 2$, $A1_4=\mp 1(s<\rightarrow>s$ or $a<\rightarrow>a$). For the transition dipole matrix elements, only the $\Delta K=0$ matrix elements were required for the transitions in $3v_2$; for the transitions in $V_2 + V_4$, the $\Delta K=\pm 1$ but also $\Delta K=\pm 2$ matrix elements were needed.

A preliminary step before any diagonalization was to get the energy and transition matrix elements of Table III and IV in terms of symmetrized basis functions in order to get both matrices in a form of symmetry blocks, according to the $D3h$ group.

IV. RESULTS

A set of computer programs based on the model described in the previous section was developed for the present analysis of line positions and intensities in the $3v_2/v_2 + v_4$ system in NH_3 . These programs are very similar in their general sequence to those worked out previously for other molecules like PH_3 . They include all the energy/ intensity possibilities of fitting and prediction as presented in Fig. 2 of Fief. (11). As a first step, these programs were used to calculate ground state energy levels on the basis of the very accurate parameters published by Urban et al. (25). The results obtained by our program were found in complete agreement with those of Table 4 of Ref. (25) and then used as a constrained entry in all our fits of the upper state. No attempt was made to fit again the ground state parameters.

The results presented hereafter will concern successively the line assignments based on the ground state combination differences method, the fitting of the upper state energies and intensities and finally the prediction of the spectrum.

Line Assignments and Upper State Energy Fit

The present assignments cover the range from 2086 to 3110 cm⁻¹. Starting with the results from Benedict et al. in 1958 (5), the line assignments of 3v₂ and v₂ + v₄ were completed as much as possible up to J'=13, increasing the number of identified lines from 516 to 1366. For the weak V₂ + V₄, 480 line assignments were added to the 320 initially reported. In the 3v₂ band, the number of line assignments were doubled (from 216 assignments to 414 in the present work). In particular, a number of lines belonging to the Q- and to the P- branch of the 3v₂s<--a component, which were wholly obscured by the CO₂ absorption in the previous work (5), are now assigned. For the fit of the upper state energies, all the lines which correspond to multiple or uncertain assignments were disregarded and finally 1213 lines (J' ≤ 12) corresponding to about 500 different upper state energy levels were included in the fit.

A set of 48 upper-state parameters, presented in Table V is retained allowing to reproduce the experimental transitions with an overall standard deviation of 0.0069 cm⁻¹. This deviation is roughly a factor 35 bigger than the experimental uncertainty estimated for strong unblended well-isolated lines. Even by taking into account the degradation of the measurement precision by pressure shift as described in section 11, a factor of nearly 16 finally represents the limitation of our model. The parameters reported in Table V are defined according to notation of Table III. No important correlations between the parameters were observed.

It should be noted that the quality of our fit is similar for the degenerate V₂ + V₄ band (r.m.s = 0.0070 cm⁻¹ for 799 transitions) and for the non-degenerate band 3v₂ (r.m.s = 0.0067 cm⁻¹ for 414 transitions). In the case of the V₂ + V₄ band the quality of the fit is roughly similar for the a<--a and sc--s components whereas the r.m.s deviation of the 3v₂s<--a component (of 0.0050 cm⁻¹) is much better than the r.m.s. deviation of the 3v₂a<--s component (of 0.0081 cm⁻¹). This effect seems to point out the limitations of our model with respect to the vibrational interactions between the 3v₂a<--s component and the bands lying just above, namely the 2v₄ band (see figure 1).

In Table V, 17 parameters concern the upper state V₂=3, and 30 the upper state V₂=V₄=1. The columns "s" in table V give the values of the parameters for the symmetric component and the columns "a-s" give the differences of the parameters between the asymmetric and symmetric components.

The Coriolis-type coupling between the 3v₂ and v₂ + v₄ bands is not very strong. Only one parameter (C₂^s=C₂^a) describing the Coriolis-type interaction in ΔK=±2, Δl₄=±1 between the two bands has been determined. Indeed, energy levels that interact by this Coriolis-type interaction in AK=±2, A₁₄=±1 approach each other quickly enough to produce an avoided

crossing between the s components of the $V_2=3$, $K'=9$ and the $v_2 = V_4=1$, $K=1$, $1' = -1$ upper states; this allows us to determine the parameter responsible for this interaction. On the contrary, the Coriolis-type parameter in $\Delta K=\pm 1$, $\Delta l_4=\pm 1$ was not found to be determinable and did not contribute to decrease the standard deviation significantly. It was therefore taken out of the adjusted parameters to fit and fixed to zero. This problem probably arised because the energy differences between the interacting levels in $\Delta K= \pm 1$, $\Delta l_4=\pm 1$ vary much less quickly with K than the interacting levels in $\Delta K= \pm 2$, $\Delta l_4=\mp 1$ so that they do not lead to avoided crossings at the observable K values. A very different situation was found in the case of the $2v_2/v_4$ system studied by Sasada et al. (26) for which all the levels belonging to the two interacting bands are lying much closer to each other and for which it was therefore possible to determine both parameters (and their rotational dependence). Nevertheless the differences between their model and ours did not allow us to use the value they determined for the Coriolis parameters in our fit.

Similar avoided crossings take place even at small values of K between energy levels within the $V_2 + V_4$ band allowing us to determine a number of "essential" resonances parameters in our fit such as the parameters q_1 and q_2 (and their rotational dependances) as well as the f_4 parameter responsible for interactions between energy levels characterized respectively by $\Delta K= \pm 1$, $\Delta l_4=\mp 2$ ($a<\rightarrow>s$), $\Delta K= \pm 2$, $\Delta l_4=\pm 2$ and $\Delta K= \pm 4$, $\Delta l_4=\mp 2$ ($s<\rightarrow>s$ or $a<\rightarrow>a$). Among those interacting levels, the particularly strong interaction in $\Delta K=\pm 1$, $\Delta l=\mp 2$ within the $V_2 + V_4$ makes some $\Delta K=\pm 2$ $a<\rightarrow>s$ or $s<\rightarrow>a$ perturbation-allowed transitions observable. We have kept the "s" and "a" notation for the upper state energy levels inspite of the rather strong mixing between these two components due to the interactions in $\Delta K=\pm 1$.

In the $v_2=v_4=1$ upper state, the sixth order parameters H_j , H_{jk} , H_{kj} and H_k were not found to be significatively different from their ground state value for neither the asymmetric nor the symmetric components. These parameters were therefore constrained to their ground state values as shown in Table V. In the $V_2=3$ upper state, these H parameters were found to exhibit large variations from their ground state values. However the differences between the asymmetric and symmetric values were not found to be significatively different from the ground state values and therefore fixed to these ground state values.

The upper state energy levels of the $3v_2 / v_2 + v_4$ system calculated using parameters from Table V are represented in function of the rotational quantum number J in Fig. 4 to illustrate the mixing of levels between the $3v_2$ and $v_2 + v_4$ bands and also within $V_2 + V_4$.

Intensity Fit

Some 726 intensity measurements were selected by disregarding lines which correspond to either multiple or uncertain assignments. The data set contains 116,144, 219

and 247 transitions from $3\nu_2 s \leftarrow a$, $3\nu_2 a \leftarrow s$, $\nu_2 + \nu_4 s \leftarrow s$ and $\nu_2 + \nu_4 a \leftarrow a$. The fit of these intensity data led to the determination of four transition dipole moments and eight Herman-Wallis corrections in the $3\nu_2$ and $\nu_2 + \nu_4$ bands. Their best values, obtained by least-square fitting, are reported in Table VI, according to the notation of Table IV. The intensity parameters are noted "s" or "a" depending whether they concern transitions originating from "s" or "a" ground state energy levels; so "s" notation is used for $3\nu_2 a \leftarrow s$, $\nu_2 + \nu_4 s \leftarrow s$ transitions and perturbed allowed $\nu_2 + \nu_4 a \leftarrow s$ transitions, "a" notation for $3\nu_2 s \leftarrow a$, $\nu_2 + \nu_4 a \leftarrow a$ transitions and perturbed allowed $\nu_2 + \nu_4 s \leftarrow a$ transitions. In Table VI the values of the "s" parameters and of the differences "a-s" between the "a" and the "s" intensity parameters which correspond to the actual fitted parameters are presented. They reproduce the experimental line intensities with a r.m.s equal to 5.66 %, quite close to the estimated uncertainty of the absolute intensity measurements (of 5%). The r.m.s deviations for the four components taken separately are 5.59 % for the 116 transitions of $3\nu_2 s \leftarrow a$, 3.70 % for the 144 transitions of $3\nu_2 a \leftarrow s$, 4.94 % for the 219 transitions of $\nu_2 + \nu_4 s, a \leftarrow s$ and 7.04 % for the 247 transitions of $\nu_2 + \nu_4 a, s \leftarrow a$.

In Table VI, the first subscripts 0 and 1 are related to $3\nu_2$ and $\nu_2 + \nu_4$ transitions respectively. All the parameters with two indices correspond to Herman-Wallis corrections defined in Table IV. In this fit, only the parameters showing a test value greater than twice the overall test value were retained as significant parameters. For $\nu_2 + \nu_4$, the Herman-Wallis corrections are especially large, coming to be of the same magnitude as the leading term for relatively low values of J and K. A trial fit floating only 9 parameters ($d_0^s, d_0^a - d_0^s, d_0^a - d_{01}^s, d_1^s, a_1^a - d_1^s, d_{11}^s, d_{11}^a, d_{12}^s, d_{12}^a - d_{12}^s$) and dropping the Herman-Wallis corrections d_{17}, d_{16} and d_{14} for the $\nu_2 + \nu_4$ band, gave a r.m.s. deviation of 30.73%.

The results of Table VI lead to derive vibrational transition moments and band strengths for the $3\nu_2$ and $\nu_2 + \nu_4$ bands. The transition moments for each component have the following values :

$$\langle \mu_v \rangle_{3\nu_2 a \leftarrow s} = |d_0^s| / \sqrt{2} = 0.002856(40) \text{ Debye} \quad (1)$$

$$\langle \mu_v \rangle_{3\nu_2 s \leftarrow a} = |d_0^a| / \sqrt{2} = 0.00496(13) \text{ Debye} \quad (2)$$

$$\langle \mu_v \rangle_{\nu_2 + \nu_4 s \leftarrow s} = |d_1^s| = 0.002358(36) \text{ Debye} \quad (3)$$

$$\langle \mu_v \rangle_{\nu_2 + \nu_4 a \leftarrow a} = |d_1^a| = 0.002182(82) \text{ Debye} \quad (4)$$

The values of the bandstrengths are presented in Table VII and compared to the only ones available from Benedict et al (5). In the case of $3\nu_2$ where the Herman-Wallis corrections are very small, the bandstrengths were calculated from the usual formula :

$$S_v^s = \frac{8113}{3} f \cdot T_0 \cdot \frac{\mu_v^2}{Q_v(T) T} \quad (5)$$

$$S_v^a = \frac{8113}{3} f \cdot T_0 \cdot \frac{\mu_v^2}{Q_v(T) T} \quad (6)$$

with $f = 2.68675 \times 10^{19}$ molecules $\text{cm}^{-3}\text{atm}^{-1}$ at $T_0 = 273.15$ K, $T = 296$ K, Q_v set to 1 and with the band centers ν from table V. From Table VII, it can be seen that the value of S_v for $3\nu_2 = 1/2(S_v^s + S_v^a) = 0.427$ (37) $\text{cm}^2\text{atm}^{-1}$ is very close to the observed value of $\Sigma Si = 0.446 \text{ cm}^2\text{atm}^{-1}$.

For $V_2 + V_4$, where the Herman-Wallis corrections are especially large, as already mentioned, we tried tentatively to use the formula (5) and (6) by replacing $\langle \mu_v \rangle$ by an effective value of the vibrational transition moment $\langle \mu_v \rangle_{\text{eff}}$ defined as :

$$\langle \mu_v \rangle_{\text{eff}} S = d_{12}^s + d_{12}^a = \langle \mu_v \rangle^s (1 + \gamma^s) \quad (7)$$

and a similar expression for $\langle \mu_v \rangle_{\text{eff}}^a$. The parameters γ^s and γ^a are defined by the ratio $d_{12}^{s,a}/d_{12}^{s,a}$ and we have $\gamma^s = 0.128(4)$ and $\gamma^a = 0.17(7)$. The two values of $S_{v,\text{eff}}$ obtained that way are given in Table VII and leads to an effective value of the vibrational bandstrength $S_{v,\text{eff}}$ for $V_2 + V_4 = 1/2(S_{v,\text{eff}}^s + S_{v,\text{eff}}^a) = 0.180$ (14) $\text{cm}^2\text{atm}^{-1}$ still slightly below the observed value of $\Sigma Si = 0.208 \text{ cm}^2\text{atm}^{-1}$.

It can be noted by comparing the results of equations (1) and (2) that the vibrational transition moment for $3\nu_2 s \leftrightarrow a$ is 1.72 times bigger than for $3\nu_2 a \leftrightarrow s$, a ratio which is not too different from the ratio 1.62 obtained by Benedict et al. (5) but differs more significantly from the ratios of transition dipole moments calculated in ref. (22). Nevertheless our results agree with the predictions of Ref. (22) where it appears that for all the overtones involving the V_2 inversion mode the vibrational transition moment for the component $s \leftrightarrow a$ is always bigger than the component $a \leftrightarrow s$. For $V_2 + V_4$ the perturbation treatment adopted by Benedict et al. (5) does not allow us to make a comparison with our values which come from a more complete treatment of the transition dipole moment matrix.

Tables VIII-XI show a comparison between measured and calculated intensities using the energy and intensity parameters from Table V and V1. For each line, they include the line assignments, the observed wavenumbers, the measured and calculated intensity, the difference between observed and calculated frequencies (presented only in 10^{-3} cm^{-1} for indication in those tables) and the difference between measured and calculated intensity. In these tables, 47 of the 74 perturbation-allowed lines $a \leftrightarrow s$ or $s \leftrightarrow a$ within $V_2 + V_4$

(indicated by an asterisk) show observed-calculated intensities bigger than $\pm 10\%$ (in a total of 107 lines in such a situation). Those lines are made observable through the relative strong interaction in $\Delta K = \pm 1$, $\Delta l = \mp 2$ within the $V_2 + V_4$ band and are therefore very important to determine the dipole moment expansion parameter d_{17} . They illustrate thus the limitation of the theoretical model used,

Results of Table V and VI were also used to generate a line-by-line frequency and intensity prediction of NH_3 due to the $3\nu_2/\nu_2 + \nu_4$ system for all the transitions with $J' \leq 13$ with an intensity cut-off of $0.1 \cdot 10^{-6} \text{ cm}^2 \text{ atm}^{-1}$ which seems reasonable for planetary purposes. This complete data file (which has been submitted to HITRAN data base, edition 1995) is available from one of the authors by diskettes or by e-mail. A small portion of this file is reproduced in Table XII. A copy is also in deposit by the Journal. This file includes all the information needed to generate spectra at different temperatures in emission or in absorption, i.e. line assignments, observed frequencies, observed-calculated values (in 10^{-4} cm^{-1}), line intensities and upper and lower energy levels. Finally Fig. 5 presents a portion of the NH_3 absorption spectrum between 2865 and 2895 cm^{-1} near the region of the Q branch of the $3\nu_2$ band. The observed-calculated intensities reported at the top of the figure show the quality of our fit.

Beside the lines belonging to the $3\nu_2/\nu_2 + \nu_4$ system, a number of strong features appear in the spectra and have been assigned preliminary to the difference bands ($\nu_3 - \nu_2$), ($\text{VI} - \nu_2$), ($4\nu_2 - \nu_2$). A more detailed study of those bands is now under course.

v. CONCLUSIONS

The study of the $3\nu_2/\nu_2 + \nu_4$ system of NH_3 presented in this paper extends the knowledge of the very complex NH_3 spectrum in the range of 2000 to 3000 cm^{-1} . The availability of accurate position and intensity measurements from high resolution infrared spectra has permitted substantial improvement of a region that has received little attention since the very nice study of Benedict et al. in 1958 (5). Some of their results were in fact validated in the present study especially concerning the intensity ratio of the two overtone components of $3\nu_2$.

The model used in the present study points out the adequacy of the perturbation way to describe all the interactions between $3\nu_2$ and $\nu_2 + V_4$ with either ν_2 , $2\nu_2$ or V_4 . It is interesting to note that our theoretical approach which treats $3\nu_2$ and $\nu_2 + V_4$ within a dyad system allows us to reproduce line positions and intensities reasonably well. The only limitation concerns the interaction between $3\nu_2$ and $2\nu_4$ which appears through some discrepancies and anomalous values of the centrifugal distortion parameters. The number of

parameters required in our fit to achieve a reasonable agreement with the observed spectrum is relatively low (48 upper state energy parameters and 12 intensity parameters) compared to the 91 energy parameters required in the study of the $2\nu_2/\nu_4$ system (26). Moreover the quality of our fit is similar or even better than those obtained in previous works on of $^{14}\text{NH}_3$ (6) or of $^{15}\text{NH}_3$ species (4) where $3\nu_2$ and $\nu_2 + \nu_4$ were treated within a polyad including ν_2 , $2\nu_2$, $3\nu_2$, ν_4 , $\nu_2 + \nu_4$. It is probable that in the case of the $3\nu_2/\nu_2 + \nu_4$ system, the upper state energy levels are lying high enough from the top of the inversion potential barrier, so that the choice of the D_{3h} reference configuration and therefore the theoretical model adopted in our study, is more adequate than in the case of the $2\nu_2/\nu_4$ system, located in an "intermediate-case" region, near the top of the barrier.

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Table captions

“1’able 1. Experimental Conditions for the NH₃ Spectra Used in the Present Analysis.

Table 11. Sample of Individual intensity Measurements from Four Spectra.

Table 111. Upper State Energy Matrix^a for the 3v₂/ v_{2+v₄} System of NH₃.

Table IV. M-Reduced Dipole Transition Matrix^a for the 3v₂/ v_{2+v₄} System of NH₃.

Table V. Energy Parameters^a for the 3v₂/ v_{2+v₄} System of ¹⁴NH₃.

Table VI. Intensity Parameters^a for the 3v₂/ v_{2+v₄} System of ¹⁴NH₃.

Table V]]. Bandstrengths (in cm⁻² atm⁻¹) for the 3v₂/ v_{2+v₄} Bands of ¹⁴NH₃ at 296K

Table VIII. Comparison of Measured and Calculated Line Intensities in 3v₂ a <-- s

Table IX. Comparison of Measured and Calculated Line Intensities in 3v₂ s <-- a

‘1’able X. Comparison of Measured and Calculated Line Intensities in v_{2+v₄}s,a<-- s

Table X1. Comparison of Measured and Calculated Line Intensities in v_{2+v₄}a,s<-- a

Table XII. Line Positions and Intensities in the 3v₂/ v_{2+v₄} System of ¹⁴NH₃ (small portion).

FIGURE CAPTIONS

Figure 1 : The Lowest inversion-Vibration Energy Levels of $^{14}\text{NH}_3$ (from Ref. (6)).

Figure 2: The spectrum of $^{14}\text{NH}_3$ at 4 μm recorded with the McMath FTS located at Kitt Peak National Observatory using a 25 m path and 6.2 Torr of enriched Ammonia at 297.7K. The unanodized resolution is 0.011 cm^{-1} . A sample of CO was placed in another cell to provide wavenumber (cm^{-1}) calibration. The CO_2 and H_2O features arise from residual gas in the FTS chamber and external path.

Figure 3 : interaction blocks in the upper state energy matrix.

Figure 4: Upper state energy levels of $3\nu_2/\nu_2+\nu_4$

Figure 5: Comparison of observed and calculated spectra of $^{14}\text{NH}_3$ at 2415 and 2894 cm^{-1} using a 25 m path and 6.2 Torr of enriched ammonia at 297.7 K. The % residual (obs-talc) differences are plotted above. The left panel shows P branch transitions of $\nu_2 + \nu_4$ while the right panel has the Q ($J=K$) transitions of $3\nu_2$ a-s. To prepare this figure, the spectra were apodized and the line widths iterated with the positions and intensities held fixed.

Table 1. Experimental Conditions of the NH₃ Spectra Used the Present Analysis.

Run	Path (m)	Pressure (Torr)	Temperature (K)	Calibrated by CO	Measured for ^a
1	1.5	2.60	294.9		I
2	25.	1.05	295.0		V,I
3	25.	6.50	297.7	yes	I
4	73.0	0.5	297.0	yes	V
5	433.	0.43	297.3	yes	V, I
6	433.	6.20	297.4	yes	V

^aV indicates that line positions were measured and 1 that line intensities were retrieved from a run.

TABLE II
Sample of Individual Intensity Measurements from four spectra

	Positions cm⁻¹	O-av cm⁻¹	Int cm^{-2/atm}	% (0-av)		Path m	Press Torr	Temp K
av =	2402.424894	0.00016	1.053E-03	2.3	4			
	2402.424642	-0.00025	1.0263-03	-2.6		1.50	2.596	294.9
	2402.424927	0.00003	1.071E-03	1.7		433.00	0.430	297.0
	2402.424937	0.00004	1.032E-03	-2.0		25.00	1.050	295.0
	2402.425069	0.00018	1.083E-03	2.8		25.00	6.200	297.7
av =	2445.869837	0.00013	1.181E-03	1.4	4			
	2445.869643	-0.00019	1.156E-03	-2.1		433.00	0.430	297.0
	2445.869805	-0.00003	1.184E-03	0.2		25.00	1.050	295.0
	2445.869900	0.00006	1.181E-03	0.0		1.50	2.596	294.9
	2445.870002	0.00016	1.203E-03	1.9		25.00	6.200	297.7
av =	2449.351604	0.00006	1.944E-03	3.0	4			
	2449.351539	-0.00006	1.847E-03	-5.0		433.00	0.430	297.0
	2449.351557	-0.00005	1.999E-03	2.8		1.50	2.596	294.9
	2449.351617	0.00001	1.979E-03	1.8		25.00	1.050	295.0
	2449.351702	0\$000010	1.951E-03	0.4		25.00	6.200	297.7
av =	2475.908649	0.00006	2.999E-03	1.9	4			
	2475.908582	-0.00007	3.031E-03	1.1		25.00	6.200	297.7
	2475.908606	-0.00004	3.004E-03	0.2		1.50	2.596	294.9
	2475.908696	0.00005	3.056E-03	1.9		2.5.00	1.050	295.0
	2475.908711	0.00006	2.906E-03	-3.1		433.00	0.430	297.0
av =	2483.372594	0.00005	1.390E-03	1.3	4			
	2483.372540	-0.00005	1.371 E-03	-1.4		1.50	2.596	294.9
	2483.372542	-0.00005	1.412E-03	1.6		25.00	6.200	297.7
	2483.372641	0.00005	1.374E-03	-1.2		433.00	0.430	297.0
	2483.372655	0.00006	1.403E-03	0.9		2.5.00	1.050	295.0
av =	2490.634980	0.00005	3.413E-03	4.0	4			
	2490.634903	-0.00008	3.446E-03	1.0		2.5.00	6.200	297.7
	2490.634995	0.00002	3.182E-03	-6.7		433.00	0.430	297.0
	2490.634996	0.00002	3.514E-03	3.0).50	2.596	294.9
	2490.635025	0.00005	3.509E-03	2.8		2.5.00	1.050	295.0
av =	2894.294482	0.00010	2.133E-03	2.6	4			
	2894.294366	-0.00012	2.041E-03	-4.3		433.00	0.430	297.3
	2894.294447	-0.00004	2.191E-03	2.7		25.00	1.050	295.0
	2894.294488	0.00001	2.156E-03	1.1		1.50	2.596	294.9
	2894.294629	0.00015	2.144E-03	0.5		25.00	6.200	297.7

TABLE III

Upper state energy matrix^a for the system $3v_2/v_2 + v4$ of NII_3 a) diagonal^b

$$\begin{aligned} & \langle i, v, \ell_4; JK | i, v, \ell_4; JK \rangle = v_v^i + B_v^i J(J+1) + (C_v^i - B_v^i) K^2 - D_v^{J,i} J^2 (J+1)^2 - D_v^{K,i} J(J+1) K^2 \\ & - D_v^{K,i} K^4 + H_v^{J,i} J^3 (J+1)^3 + H_v^{JK,i} J^2 (J+1)^2 K^2 + H_v^{KJ,i} J(J+1) K^4 + H_v^{K,i} K^6 - 2 (C\zeta_4)_v^i K \ell_4 \\ & + \eta_v^{J,i} J(J+1) K \ell_4 + \eta^{K,i} K^3 \ell_4 + \chi^{J,i} J^2 (J+1)^2 K \ell_4 + \chi^{JK,i} J(J+1) K^3 \ell_4 + \chi^{K,i} K^5 \ell_4 \quad (i=s, a) \end{aligned}$$

b) essential resonances

$$\begin{aligned} & \langle s, v, \ell_4; JK | a, v, \ell_4; J, K \pm 3 \rangle = F_3^\pm(J, K) [q_{3v}(2K \pm 3) \pm q_3' + d_3 \ell_4] \\ & \langle a, v, \ell_4; JK | s, v, \ell_4; J, K \pm 3 \rangle = F_3^\pm(J, K) [q_{3v}(2K \pm 3) \mp q_3' + d_3 \ell_4] \\ & \langle i, v, \ell_4; JK | i, v, \ell_4; J, K \pm 6 \rangle = F_6^\pm(J, K) f_6^i \quad (i=s, a) \\ & \langle a^s, 1, 1, \pm 1; JK | s, 1, 1, \mp 1; J, K \pm 1 \rangle = (2K \pm 1) F_1^\pm(J, K) [q_1 + q_{1J} J(J+1) + q_{1K} (2K \pm 1)^2] \\ & \langle i, 1, 1, \mp 1; JK | i, 1, 1, \pm 1; J, K \pm 2 \rangle = F_2^\pm(J, K) [q_2^i + q_{2J}^i J(J+1) + q_{2K}^i (2K \pm 2)^2] \quad (i=s, a) \\ & \langle i, 1, 1, \pm 1; JK | i, 1, 1, \mp 1; J, K \pm 4 \rangle = F_4^\pm(J, K) f_4^i \quad (i=s, a) \end{aligned}$$

c) Coriolis-type coupling^b

$$\begin{aligned} & \langle s, 3, 0, 0; JK | a, 1, 1, \pm 1; J, K \pm 1 \rangle = F_1^\pm(J, K) [C_1^s \pm C_{1K}^s (2K \pm 1)] \\ & \langle a, 3, 0, 0; JK | s, 1, 1, \pm 1; J, K \pm 1 \rangle = F_1^\pm(J, K) [C_1^a \pm C_{1K}^a (2K \pm 1)] \\ & \langle i, 3, 0, 0; JK | i, 1, 1, \mp 1; J, K \pm 2 \rangle = \pm F_2^\pm(J, K) [C_2^i \pm C_{2K}^i (2K \pm 2)] \quad (i=s, a) \end{aligned}$$

$$F_1^\pm(J, K) = [J(J+1) - K(K \pm 1)]^{1/2}; F_2^\pm(J, K) = F_1^\pm(J, K) F_1^\pm(J, K \pm 1); \dots$$

a) The elements are given according to the phase conventions of Ref (24) and obey $\langle i', v'; J, K' | i, v; J, K \rangle = \langle i, v; J, K | i', v'; J, K' \rangle$

The quantum number M is dropped all over the table

b) v represents the set (v_2, v_4) equal to $(3, 0)$ and $(1, 1)$ for the upper states of $3V2$ and $V2 + V4$, respectively

TABLE IV

M-reduced dipole transition matrix^a for the system $3\nu_2/\nu_2 + \nu_4$ of NH₃

a) $3\nu_2$

$$\langle s, v = 0; JK || \mu_Z || a, 3, 0, 0; JK \rangle = \frac{1}{\sqrt{2}} [d_0^s + d_{02}^s J(J+1) + d_{04}^s K^2] K F_{00}(J K)$$

$$\langle s, v = 0; JK || \mu_Z || a, 3, 0, 0; J'K \rangle = \frac{1}{\sqrt{2}} [d_0^s + d_{01}^s m + d_{03}^s m^2 + d_{04}^s K^2] F_{10}(m K)$$

$$\langle a, v = 0; JK || \mu_Z || s, 3, 0, 0; JK \rangle = \frac{1}{\sqrt{2}} [d_0^a + d_{02}^a J(J+1) + d_{04}^a K^2] K F_{00}(J K)$$

$$\langle a, v = 0; JK || \mu_Z || s, 3, 0, 0; J'K \rangle = \frac{1}{\sqrt{2}} [d_0^a + d_{01}^a m + d_{03}^a m^2 + d_{04}^a K^2] F_{10}(m K)$$

b) $\nu_2 + \nu_4$

$$\langle i, v = 0; JK || \mu_Z || i, 1, 1, * 1; J, K \pm 1 \rangle = \pm \frac{1}{2} [d_1^i \pm d_{12}^i (2K \pm 1) + d_{13}^i J(J+1) + d_{15}^i (2K \pm 1)^2] F_{01}^\pm(J K)$$

$$\begin{aligned} \langle i, v = 0; JK || \mu_Z || i, 1, 1, \pm 1; J', K \pm 1 \rangle = & \pm \frac{1}{2} [d_1^i + d_{11}^i m \pm d_{12}^i (2K \pm 1) + d_{14}^i m^2 + d_{15}^i (2K \pm 1)^2 \\ & \pm d_{16}^i m (2K \pm 1)] F_{11}^\pm(m K) \end{aligned} \quad (i = s, a)$$

$$\langle s, v = 0; JK || \mu_Z || a, 1, 1, \pm 1; J, K \mp 2 \rangle = -\frac{1}{2} [d_{17}^s \pm d_{19}^s (2K \mp 2)] F_{02}^\mp(J K)$$

$$\langle s, v = 0; JK || \mu_Z || a, 1, 1, \pm 1; J', K \mp 2 \rangle = \frac{1}{2} [d_{17}^s + d_{18}^s m \pm d_{19}^s (2K \mp 2)] F_{12}^\mp(m K)$$

$$\langle a, v = 0; JK || \mu_Z || s, 1, 1, \pm 1; J, K \mp 2 \rangle = \frac{1}{2} [d_{17}^a \pm d_{19}^a (2K \mp 2)] F_{02}^\mp(J K)$$

$$\langle a, v = 0; JK || \mu_Z || s, 1, 1, * 1; J', K \mp 2 \rangle = \frac{1}{2} [d_{17}^a + d_{18}^a m \pm d_{19}^a (2K \mp 2)] F_{12}^\mp(m K)$$

a $\langle ||\mu_Z|| \rangle$ is defined according to the notation of Ref (24), Eq.2.

The first subscripts O and 1 in the intensity coefficients are related to $3\nu_2$ and $\nu_2 + \nu_4$, respectively

$v = O$ represents the set $(\nu_2, \nu_4, \ell_4) \equiv (O, O, O)$ for the ground state

$m = J + 1$ and $-J$ for $J' = J+1$ (R branch) and $J - 1$ (P branch), respectively

F functions are expressed in terms of J, m and K in Table XIV of Ref (24).

TABLE V
Energy parameters for the system $3\nu_2/\nu_2 + \nu_4$ of $^{14}\text{NH}_3$

	$3\nu_2$		$\nu_2 - t \nu_4$	
	s	a-s	s	a - s
a) diagonal				
v	2384.1477 (57)	511.3652 (69)	2540.5287 (33)	45.6030 (48)
B,	9.49981 (29)	-0.30293 (25)	10.31504 (12)	-0.21041 (18)
C"	6.19169 (39)	0.10411 (28)	6.01800 (15)	0.090039 (22)
$D_v^J \times 10^3$	-0.2639 (42)	0.0086 (19)	1.3122 (11)	-0.4593 (14)
$D_v^{JK} \times 10^2$	0.1282 (10)	-0.00846 (36)	-0.27747 (69)	0.12625 (87)
$D_v^K \times 10^3$	-0.9440 (78)	0.1198 (36)	1.6843 (75)	-0.8674 (78)
$H_v^J \times 10^6$	-0.500 (18)	fixed ^b	fixed ^b	fixed ^b
$H_v^{JK} \times 10^5$	0.1744 (60)	fixed ^b	fixed ^b	fixed ^b
$H_v^{KJ} \times 10^5$	-0.2035 (72)	fixed ^b	fixed ^b	fixed ^b
$H_v^K \times 10^6$	0.780 (36)	fixed ^b	fixed ^b	fixed ^b
$(C\zeta_4)_v$			-1.30276 (51)	-0.18416 (48)
$\eta_v^J \times 10^2$			-0.211 1(30)	- 0.1527(19)
$\eta_v^K \times 10^2$			0.1184 (33)	0.1964 (26)
$X^{JK} \times 10^5$			-0.87 (14)	
$X^K \times 10^5$			0.88 (14)	
b) essential				
$q_{3\nu} \times 10^3$	-0.278 (26)		-0.2258 (33)	
q_1			0.11074 (26)	
$q_{1J} \times 10^3$			-0.1316(26)	
$q_{1K} \times 10^4$			0.636 (44)	
q_2		-	0.124686 (90)	0.017438 (78)
$q_{2J} \times 10^4$			-0.8220 (84)	0.
$q_{2K} \times 10^4$			-0.632 (34)	0.
$f_4 \times 10^4$			0.1718 (66)	0.044 (lo)
c) Coriolis				
	$C_2^s = C_2^a = 0.01158 (66)$			
Number of transitions	414		799	
r.m.s.d. in 10^{-3} cm ⁻¹	6.74		7.01	

a) The quoted errors represent three standard deviations

b) fixed to the ground state values determined in Ref (25)

TABLE VI

Intensity parameters for the system $3\nu_2/\nu_2 + \nu_4$ of $^{14}\text{NH}_3$

	3V2	$\nu_2 + \nu_4$		
	d^s	$d^a - d^s$	d^s	$d^a - d^s$
$d_0 \times 10^2$	-0.4039 (57)	-0.298 (13)		
$d_{01} \times 10^3$	o.	-0.208 (16)		
$d_1 \times 10^2$			0.2358 (36)	-0.0176 (46)
$d_{11} \times 10^3$			-0.5131 (84)	-0.135(13)
$d_{12} \times 10^3$			0.3021 (51)	0.0658 (75)
$d_{14} \times 10^5$			-0.99 (lo)	o.
$d_{16} \times 10^5$			0.554 (63)	o.
$d_{17} \times 10^3$			-0.1677 (36)	o.
Number of data	260		466	
r.m.s.d. in %	4.63		6.16	

a The quoted errors represent three standard deviations.

$d_0^s, d_{01}^s, d_1^s, \dots$ are related to transitions going from ground states levels; $d_0^a, d_{01}^a, d_1^a, \dots$

are related to transitions going from ground state a levels.

The signs of intensity parameters are correlated to those of the energy parameters given in Table Iv.

Table VII: Bandstrengths (in $\text{cm}^{-2} \text{atm}^{-1}$) for the $3\nu_2$ and $\nu_2 + \nu_4$ bands of $^{14}\text{NH}_3$.

	Band Centers (cm^{-1})	From present work	From Benedict et al. (5)
S_{ν^s} ($3\nu_2$ a \leftarrow s)	2895.52	0.244(7)	0.20 (1)
S_{ν^a} ($3\nu_2$ s \leftarrow a)	2384.15	0.61 (3)	0.44 (5)
$S_{\nu,\text{eff}}^s$ ($\nu_2 + V4$ Se-s)	2540.53	0.186(3)	0.06
$S_{\nu,\text{eff}}^a$ ($\nu_2 + V4$ a \leftarrow a)	2586.13	0.174(25)	0.06

Table VII.

Comparison of Measured and Calculated Line Intensities in $3v_2 a \leftarrow s$

(I)	Transition				Intensity data from							
	(II)	(III)	(IV)	(V)	experiment	present analysis	(VI)	(VII)	(VIII)	(IX)		
1	(Q)P (1, 0,s)	O A2"	1 a 0 0	3nu2	2875.63201	0.1444E02	0.1523E-02	-5.48	9			
2	(Q)P (2, 1,s)	1 E'	3 a 1 0	3nu2	2855.07401	0.9210E-03	0.9519E-03	-3.35	7			
3	(Q)Q (1, 1,s)	1 E'	3 a 1 0	3nu2	2894.83981	0.1124E-02	0.1171E-02	-4.18	7			
4	(Q)P (3, 0,s)	2 A2"	3 a 0 0	3nu2	2831.46648	0.2638E-02	0.2776E-02	-5.23	1			
5	(Q)R (1, 0,s)	2 A2"	3 a 0 0	3nu2	2930.81440	0.2816E-02	0.3105E02	'10.25	1			
6	(Q)P (3, 1,s)	2 E'	5 a 1 0	3nu2	2832.26161	0.1240E-02	0.1257E-02	-1.33	2			
7	(Q)Q (2, 1,s)	2 E'	5 a 1 0	3nu2	2891.85963	0.5551E-03	0.5356E-03	3.51	2			
8	(Q)R (1, 1,s)	2 E'	5 a 1 0	3nu2	2931.62534	0.1098E-C12	0.1186E-02	'8.00	2			
9	(Q)P (3, 2,s)	2 E"	5 a 2 0	3nu2	2834.66828	0.8175E-03	0.8296E-03	-1.49	6			
10	(Q)Q (2, 2,s)	2 E"	5 a 2 0	3nu2	2894.29448	0.2134E-02	0.2264E-02	'6.07	6			
11	(Q)P (4, 1,s)	3 A2'	4 a 3 0	3nu2	2814.41531	0.1259E-02	0.1287E-02	-2.20	6			
12	(Q)Q (3, 3,s)	3 A2'	4 a 3 0	3nu2	2893.88488	0.5275E-02	0.5839E-02	'10.70	6			
13	(Q)P (4, 1,s)	3 E'	7 a 1 0	3nu2	2808.08795	0.1197E-02	0.1191E-02	0.48	-2			
14	(Q)Q (3, 1,s)	3 E'	7 a 1 0	3nu2	2887.45768	0.2714E-03	0.2802E-03	-3.23	-2			
15	(Q)R (2, 1,s)	3 E'	7 a 1 0	3nu2	2947.05553	0.1606E-02	0.1746E-02	'8.75	-2			
16	(Q)P (4, 2,s)	3 E"	7 a 2 0	3nu2	2810.43418	0.9830E-03	0.1007E-02	-2.40	0			
17	(Q)Q (3, 2,s)	3 E"	7 a 2 0	3nu2	2889.84118	0.1115E-02	0.1184E-02	-6.18	0			
18	(Q)R (2, 2,s)	3 E"	7 a 2 0	3nu2	2949.46738	0.1077E02	0.1153E-02	-7.09	0			
19	(Q)P (5, 3,s)	4 A2'	4 a 3 0	3nu2	2788.77510	0.1413E-02	0.1440E-02	-1.89	-2			
20	(Q)Q (4, 3,s)	4 A2'	4 a 3 0	3nu2	2887.96074	0.2861E-02	0.3054E-02	-6.76	-1			
21	(Q)R (3, 3,s)	4 A2'	4 a 3 0	3nu2	2967.43030	0.1834E-02	0.1996E-02	'8.82	-1			
22	(Q)P (5, 0,s)	4 A2°	5 a 0 0	3nu2	2781.90137	0.1878E-02	0.1910E-02	'1.72	-5			
23	(Q)R (3, 0,s)	4 A2"	5 a 0 0	3nu2	2960.30533	0.3473E-02	0.3868E-02	-11.38	-5			
24	(Q)P (5, 1,s)	4 E'	9 a 1 0	3nu2	2782.65152	0.9256E-03	0.9337E-03	-0.88	-5			
25	(Q)R (3, 1,s)	4 E'	9 a 1 0	3nu2	2961.08315	0.1729E-02	0.1847E-02	-6.80	-5			
26	(Q)P (5, 4,s)	4 E"	8 a 4 0	3nu2	2794.31670	0.4624E-03	0.4601E-03	0.50	6			
27	(Q)Q (4, 4,s)	4 E"	8 a 4 0	3nu2	2893.61139	0.2863E-02	0.3087E-02	-7.82	6			
28	(Q)P (5, 2,s)	4 E"	9 a 2 0	3nu2	2784.92245	0.8797E-03	0.8627E-03	1.93	-4			
29	(Q)Q (4, 2,s)	4 E"	9 a 2 0	3nu2	2884.03044	0.6273E-03	0.6195E-03	1.25	-4			
30	(Q)R (3, 2,s)	4 E"	9 a 2 0	3nu2	2963.43733	0.1453E-02	0.1561E-02	-7.41	-4			
31	(Q)P (6, 3,s)	5 A2'	6 a 3 0	3nu2	2761.95548	0.1128E-02	0.1126E-02	0.19	-5			
32	(Q)Q (5, 3,s)	5 A2'	6 a 3 0	3nu2	2880.75733	0.1463E-02	0.1532E-02	-4.75	-5			
33	(Q)R (4, 3,s)	5 A2'	6 a 3 0	3nu2	2979.94292	0.2293E-02	0.2490E-02	-8.58	-5			
34	(Q)P (6, 5,s)	5 E'	10 a 5 0	3nu2	2774.37595	0.3106E-03	0.3068E-03	1.23	5			
35	(Q)Q (5, 5,s)	5 E'	10 a 5 0	3nu2	2893.47677	0.4028E-02	0.2852E-02	29.19	6			
36	(Q)P (6, 1,s)	5 E'	11 a 1 0	3nu2	2756.07188	0.6506E-03	0.6315E-03	2.94	-4			
37	(Q)Q (5, 1,s)	5 E'	11 a 1 0	3nu2	2874.72787	0.7322E04	0.7361E-04	-0.53	-4			
38	(Q)R (4, 1,s)	5 E'	11 a 1 0	3nu2	2973.79000	0.1522E-02	0.1613E-02	-6.01	-4			
39	(Q)Q (5, 4,s)	5 E"	10 a 4 0	3nu2	2886.21132	0.1466E-02	0.1548E-02	-5.59	-3			
40	(Q)R (4, 4,s)	5 E"	10 a 4 0	3nu2	2985.50603	0.7690E-03	0.7962E-03	-3.53	-3			
41	(Q)P (6, 2,s)	5 E"	1 a 2 0	3nu2	2758.25340	0.6266E-03	0.6095E-03	2.73	-4			
42	(Q)Q (5, 2,s)	5 E"	1 a 2 0	3nu2	2876.96403	0.3053E-03	0.3109E-03	-1.84	-4			
43	(Q)R (4, 2,s)	5 E"	1 a 2 0	3nu2	2976.07225	0.1427E-02	0.1491E-02	-4.50	-4			
44	(Q)P (7, 3,s)	6 A2'	6 a 3 0	3nu2	2734.09631	0.7583E-03	0.7229E-03	4.67	-2			
45	(Q)Q (6, 3,s)	6 A2'	6 a 3 0	3nu2	2872.39986	0.7077E-03	0.7238E-03	2.27	-2			
46	(Q)R (5, 3,s)	6 A2'	6 a 3 0	3nu2	2991.20183	0.2032E-02	0.2169E-02	6.74	-2			
47	(Q)P (7, 6,s)	6 A2°	6 a 6 0	3nu2	2754.59778	0.3893E-03	0.3832E-03	1.57	5			
48	(Q)P (7, 0,s)	6 A2°	7 a 0 0	3nu2	2727.79986	0.7665E-03	0.7534E-03	1.71	0			
49	(Q)R (5, 0,s)	6 A2°	7 a 0 0	3nu2	2984.55131	0.2321E-02	0.2455E-02	-5.79	0			
50	(Q)P (7, 5,s)	6 E'	12 a 5 0	3nu2	2745.94410	0.2963E-03	0.2895E-03	2.28	-4			
51	(Q)Q (6, 5,s)	6 E'	12 a 5 0	3nu2	2884.58831	0.1283E-02	0.1345E-02	-4.84	-4			
52	(Q)R (5, 5,s)	6 E'	12 a 5 0	3nu2	3003.68819	0.5509E-03	0.5922E-03	-7.49	-4			
53	(Q)P (7, 1,s)	6 E'	13 a 1 0	3nu2	2728.48681	0.3949E-03	0.3757E-03	4.86	0			
54	(Q)Q (6, 1,s)	6 E'	13 a 1 0	3nu2	2866.62103	0.3238E-04	0.3479E-04	-7.44	-1			
55	(Q)R (5, 1,s)	6 E'	13 a 1 0	3nu2	2985.27732	0.1172E-02	0.1215E-02	-3.71	0			
56	(Q)P (7, 4,s)	6 E"	12 a 4 0	3nu2	2739.17515	0.3483E-03	0.3383E-03	2.87	-4			
57	(Q)Q (6, 4,s)	6 E"	12 a 4 0	3nu2	2877.62610	0.7053E-03	0.7305E-03	-3.58	-4			
58	(Q)R (5, 4,s)	6 E"	12 a 4 0	3nu2	2996.55785	0.8567E-03	0.9129E-03	-6.56	-4			
59	(Q)P (7, 2,s)	6 E"	13 a 2 0	3nu2	2730.56675	0.3848E-03	0.3717E-03	3.41	-1			
60	(Q)Q (6, 2,s)	6 E"	13 a 2 0	3nu2	2868.76369	0.1427E-02	0.1469E-03	-2.95	-1			
61	(Q)R (5, 2,s)	6 E"	13 a 2 0	3nu2	2987.47460	0.1140E-02	0.1174E-02	-2.94	-1			
62	(Q)P (8, 3,s)	7 A2'	8 a 3 0	3nu2	2705.35752	0.4157E-03	0.4002E-03	3.73	1			
63	(Q)R (6, 3,s)	7 A2'	8 a 3 0	3nu2	3001.32709	0.1487E-02	0.1550E-02	-4.24	1			
64	(Q)P (8, 6,s)	7 A2"	7 a 6 0	3nu2	2724.76661	0.3370E-03	0.3311E-03	1.75	-6			
65	(Q)Q (7, 6,s)	7 A2"	7 a 6 0	3nu2	2883.08816	0.1952E-02	0.2080E-02	'6.54	-6			

Note.(I)Serial number ;(II)Assignment ;(III)Identification of the upper level ;(IV)Vibrational band
 (V)Observed wavenumber in cm⁻¹; (VI)So in cm⁻² atm⁻¹ at 296K; (VII)Sc in cm⁻² atm⁻¹ at 296K;
 (VIII)So-Sc/So in %; (Obs-Cal)wavenumber in 10⁻³ cm⁻¹

Table VIII_Continued

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(I)	(II)	Transition					Intensity data from			
		(III)		(IV)	(V)	(VI)	(VII)	(VIII)	(IX)	
66	(Q)R 6, 6,s	7 A 2°	7 a 6 0	3nu2	3021.97201	0.7658E-03	0.8248E-03	-7.71	-6	
67	(Q)P 8, 7,s	7 E'	13 a 7 0	3nu2	2734.98856	0.1158E-03	0.1123E-03	3.01	5	
68	(Q)Q 7, 7,s	7 E'	13 a 7 0	3nu2	2893.63376	0.1647E-02	0.1796E-02	-9.06	5	
69	(Q)P 8, 5,s	7 E'	14 a 5 0	3nu2	2716.57182	0.1946E-03	0.1890E-03	2.86	-4	
70	(Q)Q 7, 5,s	7 E'	14 a 5 0	3nu2	2874.62442	0.5744E-03	0.5910E-03	-2.88	-4	
71	(Q)R 6, 5,s	7 E'	14 a 5 0	3nu2	3013.26859	0.5936E-03	0.6223E-03	-4.84	-4	
72	(Q)P 8, 1,s	7 E'	15 a 1 0	3nu2	2700.04931	0.2152E-03	0.1987E-03	7.66	2	
73	(Q)Q 7, 1,s	7 E'	15 a 1 0	3nu2	2857.52915	0.1401E-04	0.1532E-04	-9.38	2	
74	(Q)R 6, 1,s	7 E'	15 a 1 0	3nu2	2995.66354	0.7798E-03	0.8047E-03	-3.20	2	
75	(Q)P 8, 4,s	7 E"	14 a 4 0	3nu2	2710.16301	0.2092E-03	0.1979E-03	5.39	0	
76	(Q)R 6, 4,s	7 E"	14 a 4 0	3nu2	3006.44956	0.7087E-03	0.7261E-03	-2.46	0	
77	(Q)P 8, 2,s	7 E"	15 a 2 0	3nu2	2702.01662	0.2139E-03	0.1996E-03	6.66	2	
78	(Q)Q 7, 2,s	7 E"	15 a 2 0	3nu2	2859.56718	0.6488E-04	0.6469E-04	0.29	2	
79	(Q)R 6, 2,s	7 E"	15 a 2 0	3nu2	2997.76421	0.7867E-03	0.7965E-03	-1.24	2	
80	(Q)P 9, 3,s	8 A2'	8 a 3 0	3nu2	2675.90149	0.2123E-03	0.1951E-03	8.09	7	
81	(Q)Q 8, 3,s	8 A2'	8 a 3 0	3nu2	2852.79256	0.1310E-03	0.1299E-03	0.83	7	
82	(Q)R 7, 3,s	8 A2'	8 a 3 0	3nu2	3010.45831	0.9755E-03	0.9541E-03	2.19	7	
83	(Q)P 9, 6,s	8 A2°	8 a 6 0	3nu2	2694.13687	0.2056E-03	0.1974E-03	4.44	-3	
84	(Q)Q 8, 6,s	8 A2°	8 a 6 0	3nu2	2871.74253	0.8130E-03	0.8453E-03	-3.97	-3	
85	(Q)R 7, 6,s	8 A2"	8 a 6 0	3nu2	3030.06409	0.7534E-03	0.7929E-03	5.24	-3	
86	(Q)P 9, 0,s	8 A2°	9 a 0 0	3nu2	2670.31603	0.1975E-03	0.1872E-03	5.20	2	
87	(Q)R 7, 0,s	8 A2"	9 a 0 0	3nu2	3004.42371	0.1014E-02	0.9443E-03	6.87	2	
88	(Q)P 9, 7,s	8 E'	15 a 7 0	3nu2	2703.74659	0.9332E-04	0.8873E-04	4.92	-8	
89	(Q)R 7, 7,s	8 E'	15 a 7 0	3nu2	3040.35401	0.2524E-03	0.2696E-03	-6.80	-8	
90	(Q)P 9, 5,s	8 E'	16 a 5 0	3nu2	2686.43501	0.1055E-03	0.1009E-03	4.38	2	
91	(Q)R 7, 5,s	8 E'	16 a 5 0	3nu2	3021.79668	0.4536E-03	0.4519E-03	0.38	2	
92	(Q)P 9, 1,s	8 E'	17 a 1 0	3nu2	2670.92511	0.1080E-03	0.9411E-04	12.87	2	
93	(Q)R 7, 1,s	8 E'	17 a 1 0	3nu2	3005.08217	0.4843E-03	0.4732E-03	2.29	2	
94	(Q)P 9, 8,s	8 E"	15 a 8 0	3nu2	2715.55588	0.6639E-04	0.6189E-04	6.78	4	
95	(Q)Q 8, 8,s	8 E"	15 a 8 0	3nu2	2893.93831	0.1169E-02	0.1253E-02	-7.22	5	
96	(Q)P 9, 4,s]	8 E"	16 a 4 0	3nu2	2680.41482	0.1053E-03	0.9974E-04	5.28	5	
97	(Q)Q 8, 4,s]	8 E"	16 a 4 0	3nu2	2857.48480	0.1293E-03	0.1309E-03	1.24	5	
98	(Q)R 7, 4,s]	8 E"	16 a 4 0	3nu2	3015.32037	0.4662E-03	0.4724E-03	-1.33	5	
99	(Q)P 9, 2,s]	8 E"	17 a 2 0	3nu2	2672.77013	0.1048E-03	0.9551E-04	8.87	4	
1 %	(Q)Q 8, 2,s]	8 E"	17 a 2 0	3nu2	2849.52497	0.2618E-04	0.2640E-04	-0.82	4	
101	(Q)R 7, 2,s;	8 E"	17 a 2 0	3nu2	3007.07544	0.4918E-03	0.4756E-03	3.29	4	
102	(Q)O 9, 9,s;	9 A2'	8 a 9 0	3nu2	2894.40293	0.1485E-02	0.1620E-02	-9.07	5	
103	(Q)Q 9, 3,s;	9 A2'	10 a 3 0	3nu2	2841.84783	0.5662E-04	0.4888E-04	13.68	1	
104	(Q)R 8, 3,s;	9 A2'	10 a 3 0	3nu2	3018.73877	0.5348E-03	0.5165E-03	3.42	1	
105	(Q)Q 9, 6,s;	9 A2°	9 a 6 0	3nu2	2859.61961	0.3144E-03	0.3171E-03	-0.85	5	
106	(Q)R 8, 6,s;	9 A2"	9 a 6 0	3nu2	3037.22537	0.5176E-03	0.5253E-03	-1.49	6	
107	(Q)Q 9, 7,s;	9 E'	17 a 7 0	3nu2	2868.97261	0.2611E-03	0.2729E-03	-4.53	-2	
108	(Q)R 8, 7,s;	9 E'	17 a 7 0	3nu2	3046.93493	0.2326E-03	0.2367E-03	-1.75	-2	
109	(Q)Q 9, 5,s;	9 E'	18 a 5 0	3nu2	2852.11784	0.9107E-04	0.9035E-04	0.79	8	
110	(Q)R 8, 5,s;	9 E'	18 a 5 0	3nu2	3029.42690	0.2712E-03	0.2678E-03	1.24	8	
111	(Q)R 8, 1,s;	9 E'	19 a 1 0	3nu2	3013.67940	0.2563E-03	0.2488E-03	2.94	-1	
112	(Q)Q 9, 8,s	9 E"	17 a 8 0	3nu2	2880.45006	0.4465E-03	0.4684E-03	-4.90	-10	
113	(Q)R 8, 8,s	9 E"	17 a 8 0	3nu2	3058.83233	0.1594E-03	0.1656E-03	-3.87	-10	
114	(Q)Q 9, 4,s	9 E"	18 a 4 0	3nu2	2846.25185	0.5024E-04	0.4923E-04	2.00	7	
115	(Q)R 8, 4,s	9 E"	18 a 4 0	3nu2	3023.32157	0.2708E-03	0.2644E-03	2.38	7	
116	(Q)R 8, 2,s	9 E"	19 a 2 0	3nu2	3015.55553	0.2645E-03	0.2526E-03	4.50	0	
117	(Q)Q 10, 9,s	10 A2'	8 a 9 0	3nu2	2879.31234	0.5229E-03	0.5558E-03	-6.29	-13	
118	(Q)R 9, 9,s	10 A2'	8 a 9 0	3nu2	3077.40663	0.1722E-03	0.1913E-03	-11.07	-13	
119	(Q)Q 10, 3,s	10 A2'	10 a 3 0	3nu2	2830.40959	0.1749E-04	0.1697E-04	2.95	0	
120	(Q)R 9, 3,s	10 A2'	10 a 3 0	3nu2	3026.33768	0.2741E-03	0.2489E-03	9.20	1	
121	(Q)Q 10, 6,s	10 A2°	10 a 6 0	3nu2	2846.90252	0.1088E-03	0.1095E-03	0.67	10	
122	(Q)R 9, 6,s	10 A2"	10 a 6 0	3nu2	3043.62375	0.2889E-03	0.2837E-03	1.81	10	
123	(Q)R 9, 0,s	10 A2°	11 a 0 0	3nu2	3021.03613	0.2556E-03	0.2331E-03	8.79	-9	
124	(Q)Q 10, 7,s	10 E'	19 a 7 0	3nu2	2855.61107	0.1004E-03	0.9411E-04	6.27	8	
125	(Q)R 9, 7,s	10 E'	19 a 7 0	3nu2	3052.72012	0.1471E-03	0.1430E-03	2.81	8	
126	(Q)R 9, 5,s	10 E'	20 a 5 0	3nu2	3036.32436	0.1427E-03	0.1364E-03	4.41	7	
127	(Q)R 9, 1,s	10 E'	21 a 1 0	3nu2	3021.61393	0.1319E-03	0.1175E-03	10.95	-8	
128	(Q)Q 10, 10,s	10 E"	13 a 10 0	3nu2	2895.03687	0.4594E-03	0.4863E-03	-5.86	7	
129	(Q)Q 10, 8,s	10 E"	19 a 8 0	3nu2	2866.30743	0.1568E-03	0.1611E-03	-2.77	-2	
130	(Q)Q 10, 4,s	10 E"	20 a 4 0	3nu2	2834.47719	0.1847E-04	0.1706E-04	7.65	1	
131	(Q)R 9, 4,s	10 E"	20 a 4 0	3nu2	3030.61569	0.1468E-03	0.1301E-03	11.39	1	
132	(Q)R 9, 2,s	10 E"	21 a 2 0	3nu2	3023.36392	0.1356E-03	0.1201E-03	11.42	-6	
133	(Q)R 10, 9,s	11 A2'	10 a 9 0	3nu2	3080.87382	0.2172E-03	0.1397E-03	35.70	1	
134	(Q)P 12, 3,s	11 A2'	12 a 3 0	3nu2	2585.11980	0.1275E-04	0.1165E-04	8.63	-15	
135	(Q)R 10, 3,s	11 A2'	12 a 3 0	3nu2	3033.41679	0.1242E-03	0.1073E-03	13.58	-15	
136	(Q)P 12, 6,s	11 A2'	11 a 6 0	3nu2	2599.39000	0.1543E-04	0.1488E-04	3.59	3	

Table VIII.—Continued

(I)	Transition					Intensity data from			
	(II)		(III)		(IV)	experiment		present analysis	
	(VI)	(VII)	(VIII)	(IX)					
137 (Q)Q (11, 6,s)	11	A2"	11	a 6 0	3nu2	2833.78282	0.3413E-04	0.3479E-04 -1.94 3	
138 (Q)R (10, 6,s)	11	A2°	11	a 6 0	3nu2	3049.43715	0.1372E-03	0.1316E-03 4.11 3	
139 (Q)Q (11 11,s)	11	E'	13	a11 0	3nu2	2895.85028	0.2593E-03	0.2722E-03 -4.98 12	
140 (Q)R (10 7,s)	11	E'	21	a 7 0	3nu2	3057.89001	0.7831E-04	0.7034E-04 10.18 9	
141 (Q)Q (11 10,s)	11	E"	14	a10 0	3nu2	2878.29795	0.1510E-03	0.1529E-03 -1.28 -15	
142 (O)O (11 8,s)	11	E"	21	a 8 0	3nu2	2851.70737	0.5198E-04	0.5097E-04 1.95 9	
143 (Q)R (10, 8,s)	11	E"	21	a 8 0	3nu2	3068.26752	0.7570E-04	0.7301E-04 3.55 9	
144 (Q)R (10, 40s)	11	E"	22	a 4 0	3nu2	3037.37570	0.7553E-04	0.5695E-04 24.60 -8	

Table IX.

Comparison of Measured and Calculated Line Intensities in $3\nu_2$ s<-- a

(I)	(II)	Transition				Intensity data from			
		(111)	(IV)	(V)	(VI)	experiment	present analysis	(VII)	(VIII)
1	(Q)R (0, 0,a)	1 A2'	1 s 0 0 3nu2	.2402.35896	0.4619E-02	0.4463E-02	3.37	4	
2	(Q)P (2, 1,a)	1 E"	1 s 1 0 3nu2	2343.13440	0.2395E-02	0.2077E-02	13.26	5	
3	(Q)Q (1, 1,a)	1 E"	1 s 1 0 3nu2	2382.88025	0.3317E-02	0.2896E-02	12.71	5	
4	(Q)P (3, 2,a)	2 E'	1 s 2 0 3nu2	2322.72884	0.1873E-02	0.1696E-02	9.47	4	
5	(Q)O (2, 2,a)	2 E'	1 s 2 0 3nu2	2382.32528	0.6223E-02	0.5597E-02	10.05	4	
6	(Q)Q (2, 1,a)	2 E"	1 s 1 0 3nu2	2381.13237	0.1515E-02	0.1325E-02	12.53	0	
7	(Q)R (1, 1,a)	2 E"	1 s 1 0 3nu2	2420.87830	0.3744E-02	0.3300E-02	11.85	0	
8	(Q)P (.4, 0,a)	3 A2'	1 s 0 0 3nu2	2298.88455	0.5080E-02	0.4772E-02	6.06	-3	
9	(Q)R (.2, 0,a)	3 A2'	1 s 0 0 3nu2	2437.76S49	0.1258E-01	0.1137E-01	9.58	-3	
10	(Q)P (.4, 3,a)	3 A2'	1 s 3 0 3nu2	2302.26532	0.2792E-02	0.2457E-02	11.99	4	
11	(Q)Q (.3, 3,a)	3 A2"	1 s 3 0 3nu2	2381.69542	0.1609E-01	0.1444E-01	10.27	4	
12	(Q)P (.4, 2,a)	3 E'	1 s 2 0 3nu2	2300.35000	0.2077E-02	0.1924E-02	7.38	-1	
13	(Q)Q (.3, 2,a)	3 E'	1 s 2 0 3nu2	2379.71926	0.3272E-02	0.2930E-02	10.46	-1	
14	(Q)P (.4, 1,a)	3 E"	1 s 1 0 3nu2	2299.24542	0.2449E-02	0.2278E-02	7.00	-3	
15	(Q)Q (.3, 1,a)	3 E"	1 s 1 0 3nu2	2378.57816	0.7223E-03	0.6937E-03	3.96	-3	
16	(Q)R (.2, 1,a)	3 E"	1 s 1 0 3nu2	2438.14735	0.5125E-02	0.5148E-02	-0.44	-3	
17	(Q)P (.5, 3,a)	4 A2"	1 s 3 0 3nu2	2279.09260	0.2764E-02	0.2565E-02	7.19	-2	
18	(Q)Q (.4, 3,a)	4 A2°	1 s 3 0 3nu2	2378.23141	0.8260E-02	0.7560E-02	8.47	-2	
19	(Q)R (.3, 3,a)	4 A2°	1 s 3 0 3nu2	2457.66142	0.6941E-02	0.6212E-02	10.51	-2	
20	(Q)P (.5, 4,a)	4 E'	1 s 4 0 3nu2	2281.74801	0.9221E-03	0.8189E-03	11.19	5	
21	(Q)Q (.4, 4,a)	4 E'	1 s 4 0 3nu2	2380.99309	0.8708E-02	0.7631E-02	12.37	5	
22	(Q)P (.5, 2,a)	4 E'	2 s 2 0 3nu2	2277.30618	0.1577E-02	0.1538E-02	2.46	-4	
23	(Q)Q (.4, 2,a)	4 E'	2 s 2 0 3nu2	2376.36996	0.1646E-02	0.1535E-02	6.77	-4	
24	(Q)R (.3, 2,a)	4 E'	2 s 2 0 3nu2	2455.73912	0.5337E-02	0.4863E-02	8.88	-4	
25	(Q)P (.5, 1,a)	4 E"	1 s 1 0 3nu2	2276.27792	0.1683E-02	0.1665E-02	1.04	-4	
26	(Q)R (.3, 1,a)	4 E"	1 s 1 0 3nu2	2454.62970	0.5619E-02	0.5758E-02	-2.47	-4	
27	(Q)P (.6, 0,a)	5 A2'	1 s 0 0 3nu2	2252.47428	0.2027E-02	0.2118E-02	-4.49	-2	
28	(Q)R (.4, 0,a)	5 A2'	1 s 0 0 3nu2	2470.06825	0.1128E-01	0.1088E-01	3.57	-2	
29	(Q)P (.6, 3,a)	5 A2"	1 s 3 0 3nu2	2255.35022	0.1901E-02	0.1867E-02	1.80	-4	
30	(Q)Q (.5, 3,a)	5 A2"	1 s 3 0 3nu2	2374.10109	0.3947E-02	0.3798E-02	3.77	-4	
31	(Q)R (.4, 3,a)	5 A2"	1 s 3 0 3nu2	2473.23984	0.8992E-02	0.8189E-02	8.93	-4	
32	(Q)P (.6, 4,a)	5 E'	1 s 4 0 3nu2	2257.78726	0.8384E-03	0.7843E-03	6.45	-2	
33	(Q)Q (.5, 4,a)	5 E'	1 s 4 0 3nu2	2376.66377	0.4057E-02	0.3832E-02	5.56	-2	
34	(Q)R (.4, 4,a)	5 E'	1 s 4 0 3nu2	2475.90865	0.3000E-02	0.2614E-02	12.86	-2	
35	(Q)P (.6, 2,a)	5 E'	2 s 2 0 3nu2	2253.71724	0.1027E-02	0.1011E-02	1.53	-3	
36	(Q)Q (.5, 2,a)	5 E'	2 s 2 0 3nu2	2372.37841	0.7899E-03	0.7713E-03	2.36	-3	
37	(Q)R (.4, 2,a)	5 E'	2 s 2 0 3nu2	2471.44212	0.5177E-02	0.4910E-02	5.16	-3	
38	(Q)P (.6, 5,a)	5 E"	1 s 5 0 3nu2	2261.18347	0.5781E-03	0.5076E-03	12.19	6	
39	(Q)Q (.5, 5,a)	5 E"	1 s 5 0 3nu2	2380.22333	0.7976E-02	0.7049E-02	11.62	6	
40	(Q)P (.6, 1,a)	5 E"	2 s 1 0 3nu2	2252.77977	0.1026E-02	0.1048E-02	-2.16	-2	
41	(Q)R (.4, 1,a)	5 E"	2 s 1 0 3nu2	2470.40638	0.5011E-02	0.5316E-02	-6.09	-2	
42	(Q)P (.7, 6,a)	6 A2'	1 s 6 0 3nu2	2240.58060	0.6755E-03	0.5878E-03	12.99	6	
43	(Q)Q (.6, 6,a)	6 A2'	1 s 6 0 3nu2	2379.39339	0.1300E-01	0.1171E-01	9.95	6	
44	(Q)P (.7, 3,a)	6 A2"	1 s 3 0 3nu2	2231.18055	0.1080E-02	0.1112E-02	-3.00	-2	
45	(Q)Q (.6, 3,a)	6 A2"	1 s 3 0 3nu2	2369.42608	0.1718E-02	0.1796E-02	-4.56	-2	
46	(Q)R (.5, 3,a)	6 A2°	1 s 3 0 3nu2	2488.17696	0.7943E-02	0.7533E-02	5.17	-2	
47	(Q)P (.7, 4,a)	6 E'	1 s 4 0 3nu2	2233.36745	0.5650E-03	0.5201E-03	7.94	-3	
48	(Q)Q (.6, 4,a)	6 E'	1 s 4 0 3nu2	2371.75868	0.1847E-02	0.1811E-02	1.95	-4	
49	(Q)R (.5, 4,a)	6 E'	1 s 4 0 3nu2	2490.63498	0.3412E-02	0.3165E-02	7.23	-4	
50	(Q)P (.7, 2,a)	6 E'	2 s 2 0 3nu2	2229.72180	0.5336E-03	0.5723E-03	-7.25	0	
51	(Q)R (.5, 2,a)	6 E'	2 s 2 0 3nu2	2466.52698	0.4069E-02	0.4080E-02	-0.27	0	
52	(Q)P (.7, 5,a)	6 E"	1 s 5 0 3nu2	2236.43352	0.4686E-03	0.4447E-03	5.09	-3	
53	(Q)Q (.6, 5,a)	6 E"	1 s 5 0 3nu2	2375.01342	0.3524E-02	0.3329E-02	5.52	-3	
54	(Q)R (.5, 5,a)	6 E"	1 s 5 0 3nu2	2494.05320	0.2356E-02	0.2049E-02	13.05	-3	
55	(Q)P (.7, 1,a)	6 E"	2 s 1 0 3nu2	2228.88824	0.5353E-03	0.5787E-03	-8.11	1	
56	(Q)R (.5, 1,a)	6 E"	2 s 1 0 3nu2	2485.57871	0.4145E-02	0.4228E-02	-2.01	1	
57	(Q)P (.8, 6,a)	7 A2'	1 s 6 0 3nu2	2215.03318	0.5167E-03	0.4700E-03	9.03	-3	
58	(Q)Q (.7, 6,a)	7 A2'	1 s 6 0 3nu2	2373.28076	0.5333E-02	0.5147E-02	3.48	-4	
59	(Q)R (.6, 6,a)	7 A2'	1 s 6 0 3nu2	2512.09349	0.3419E-02	0.3002E-02	12.19	-4	
60	(Q)P (.8, 0,a)	7 A2'	2 s 0 0 3nu2	2204.52397	0.4664E-03	0.5653E-03	-21.21	6	
61	(Q)R (.6, 0,a)	7 A2'	2 s 0 0 3nu2	2499.98952	0.5694E-02	0.5923E-02	-4.03	6	
62	(Q)P (.8, 3,a)	7 A2°	1 s 3 0 3nu2	2206.73522	0.5003E-03	0.5697E-03	-13.88	1	
63	(Q)R (.6, 3,a)	7 A2"	1 s 3 0 3nu2	2502.59466	0.5325E-02	0.5680E-02	-6.66	1	
64	(Q)P (.8, 4,a)	7 E'	1 s 4 0 3nu2	2208.64595	0.2539E-03	0.2816E-03	-10.90	-1	
65	(Q)R (.6, 4,a)	7 E'	1 s 4 0 3nu2	2504.81189	0.2740E-02	0.2657E-02	3.05	-1	

Note.(I)Serial number ;(II)Assignment;(III)Identification of the upper level;(IV)Vibrational band;
(V)Observed wavenumber in cm^{-1} ;(VI)So in $\text{cm}^{-2} \text{atm}^{-1}$ at 296K;(VII)Sc in $\text{cm}^{-2} \text{atm}^{-1}$ at 296K;
(VIII)So Sc / So in %;(Obs-Calc)wavenumber in 10^{-3} cm^{-1}

Table IX._Continued

(I)	Transition				Intensity data from					
	(11)		(111)		(IV)	(V)	experiment	present	analysis	
							(VI)	(VII)	(VIII)	(IX)
66	(Q)P (8, 2,a)	7	E'	2 s 2 0	3nu2	2205.47394	0.2495E-03	0.2844E-03	-14.00	4
67	(Q)P (8, 7,a)	7	E"	1 s 7 0	3nu2	2219.95062	0.1757E-03	0.1592E-03	9.37	6
68	(Q)Q (7, 7,a)	7	E"	1 s 7 0	3nu2	2378.51289	0.5010E-02	0.4435E-02	11.48	6
69	(Q)P (8, 5,a)	7	E"	2 s 5 0	3nu2	2211.34705	0.2554E-03	0.2687E-03	5.20	-4
70	(Q)R (6, 5,a)	7	E"	2 s 5 0	3nu2	2507.91290	0.2475E-02	0.2272E-02	8.20	-4
71	(Q)P (8, 1,a)	7	E"	4 s 1 0	3nu2	2204.7S681	0.2833E-03	0.2832E-03	0.03	6
72	(Q)R (6, 1,a)	7	E"	4 s 1 0	3nu2	2500.26544	0.2820E-02	0.2954E-02	-4.73	6
73	(Q)P (9, 6,a)	8	A2'	1 s 6 0	3nu2	2189.28482	0.2412E-03	0.2585E-03	-7.18	-3
74	(Q)R (7, 6,a)	8	A2'	1 s 6 0	3nu2	2525.06455	0.3244E-02	0.3046E-02	6.12	-3
75	(Q)P (9, 3,a)	8	A2"	2 s 3 0	3nu2	2182.19294	0.2002E-03	0.2562E-03	-27.99	4
76	(Q)R (7, 3,a)	8	A2°	2 s 3 0	3nu2	2516.62828	0.3397E-02	0.3686E-02	8.50	4
77	(Q)Q (8, 8,a)	8	E'	1 s 8 0	3nu2	2377.59377	0.3534E-02	0.3093E-02	12.48	6
78	(Q)P (9, 4,a)	8	E'	2 s 4 0	3nu2	2183.79665	0.1085E-03	0.1309E-03	-20.61	2
79	(Q)R (7, 4a)	8	E'	2 s 4 0	3nu2	2518.57801	0.1766E-02	0.1822E-02	-3.19	2
80	(Q)P (9, 2,a)	8	E'	4 s 2 0	3nu2	2181.14138	0.9965E-04	0.1255E-03	-25.91	6
81	(Q)R (7, 2,a)	8	E'	4 s 2 0	3nu2	2515.33618	0.1689E-02	0.1839E-02	-8.90	6
82	(Q)P (9, 7,a)	8	E"	1 s 7 0	3nu2	2193.58914	0.1176E-03	0.1160E-03	1.32	-4
83	(Q)Q (8, 7,a)	8	E"	1 s 7 0	3nu2	2371.46802	0.1966E-02	0.1804E-02	8.26	-4
84	(Q)R (7, 7,a)	8	E"	1 s 7 0	3nu2	2530.03024	0.1220E-02	0.1031E-02	15.50	-4
85	(Q)P (9, 5,a)	8	E"	2 s 5 0	3nu2	2186.09910	0.1139E-03	0.1322E-03	-16.09	0
86	(Q)R (7, 5,a)	8	E"	2 s 5 0	3nu2	2521.32712	0.1790E-02	0.1740E-02	2.80	0
87	(Q)R (7, 1,a)	8	E"	4 s 1 0	3nu2	2514.60030	0.1661E-02	0.1831E-02	-10.24	7
88	(Q)R (8, 6,a)	9	A2'	1 s 6 0	3nu2	2537.70591	0.2146E-02	0.2127E-02	0.89	0
89	(Q)R (8, 0,a)	9	A2'	3 s 0 0	3nu2	2528.53266	0.1705E-02	0.2018E-02	-18.38	4
90	(Q)Q (9, 9,a)	9	A2"	1 s 9 0	3nu2	2376.64975	0.4606E-02	0.3994E-02	13.28	4
91	(Q)R (8, 3,a)	9	A2"	2 s 3 0	3nu2	2530.42933	0.1855E-02	0.2103E-02	-13.37	3
92	(Q)Q (9, 8,a)	9	E'	1 s 8 0	3nu2	2369.57979	0.1134E-02	0.1159E-02	-2.19	-5
93	(Q)R (8, 8,a)	9	E'	1 s 8 0	3nu2	2547.86669	0.7906E-03	0.6645E-03	15.95	-5
94	(Q)R (8, 4,a)	9	E'	3 S " 4 0	3nu2	2532.08473	0.9847E-03	0.1075E-02	-9.14	2
95	(Q)R (8, 2,a)	9	E'	6 s 2 0	3nu2	2529.34306	0.9100E-03	0.1029E-02	-13.13	3
96	(Q)R (8, 7,a)	9	E"	1 s 7 0	3nu2	2542.08254	0.1024E-02	0.9565E-03	6.60	-2
97	(Q)R (8, 1,a)	9	E"	5 s 1 0	3nu2	2528.73047	0.8798E-03	0.1014E-02	-15.30	4
98	(Q)R (9, 6,a)	10	A2'	2 s 6 0	3nu2	2550.18484	0.1141E-02	0.1210E-02	-6.06	0
99	(Q)Q (10, 9,a)	10	A2"	1 s 9 0	3nu2	2367.62298	0.1295E-02	0.1375E-02	-6.15	-5
100	(Q)R (9, 9,a)	10	A2"	1 s 9 0	3nu2	2565.60788	0.9678E-03	0.8046E-03	16.86	-5
101	(Q)R (9, 3,a)	10	A2"	3 s 3 0	3nu2	2544.15380	0.9151E-03	0.1067E-02	-16.62	-4
102	(O)O (10, 10,a)	10	E'	1 Slo o	3nu2	2375.69604	0.1346E-02	0.1198E-02	10.96	1
103	(Q)R (9, 8,a)	10	E'	2 s 8 0	3nu2	2558.93866	0.5933E-03	0.5726E-03	3.49	9
104	(Q)R (9, 4,a)	10	E'	5 s 4 0	3nu2	2545.49402	0.4771E-03	0.5571E-03	-16.77	-3
105	(Q)R (9, 7,a)	10	E"	1 s 7 0	3nu2	2553.93339	0.6240E-03	0.6088E-03	2.44	1
106	(Q)R (9, 5,a)	10	E"	4 s 5 0	3nu2	2547.44532	0.5290E-03	0.5830E-03	-10.22	0
107	(Q)R (9, 1,a)	10	E"	6 s 1 0	3nu2	2542.81450	0.4058E-03	0.5046E-03	24.35	-3
108	(Q)R (10, 6,a)	11	A2'	3 s 6 0	3nu2	2562.67757	0.5190E-03	0.5911E-03	-13.89	-4
109	(Q)R (10, 0,a)	11	A2'	5 s 0 0	3nu2	2556.91542	0.3366E-03	0.4483E-03	-33.17	-4
110	(Q)R (10, 9,a)	11	A2"	2 s 9 0	3nu2	257S.72064	0.6835E-03	0.6133E-03	10.28	2
111	(Q)R (10, 3,a)	11	A2"	4 s 3 0	3nd2	2557.98108	0.3745E-03	0.4851E-03	-29.54	-6
112	(Q)R (10, 10,a)	11	E'	1 s 10 o	3nu2	2583.26095	0.2817E-03	0.2290E-03	18.72	-4
113	(Q)R (10, 8,a)	11	E'	2 s 8 0	3nu2	2569.99358	0.3258E-03	0.3277E-03	-0.57	5
114	(Q)R (10, 7,a)	11	E"	3 s 7 0	3nu2	2565.76100	0.2907E-03	0.3154E-03	8.51	0
115	(Q)R (10, 5,a)	11	E"	6 s 5 0	3nu2	2560.48772	0.2292E-03	0.2750E-03	-19.99	-7
116	(Q)R (11, 9,a)	12	A2"	1 s 9 0	3nu2	2585.77378	0.2973E-03	0.3390E-03	-14.03	-6

Table X.

Comparison of Measured and Calculated Line Intensities in $v_2 + v_4$, $s, a <-- s$

(I)	(II)	(III)	(IV)	(V)	Intensity data from			
					experiment	present analysis	(VII)	(VIII)
1 (P)P (1, 1,s)	O E' 1 s 0 1	nu24	2524.35005	0.2878E-03	0.2734E-03	5.01	-5	
2 (R)Q (1, 0,s)	1 A2'' 1 s 1 1	nu24	2539.32011	0.1798E-02	0.1741E-02	3.16	-3	
3 (P)P (2, 1,s)	1 E' 1 s 0 1	nu24	2505.21039	0.4963E-03	0.4759E-03	4.12	-3	
4 (P)Q (1, 1,s)	1 E' 1 s 0 1	nu24	2544.97616	0.2796E-03	0.2650E-03	5.23	-3	
5 (P)P (2, 2,s)	1 E'' 2 s 1-1	nu24	2509.45551	0.7038E-03	0.6605E-03	6.15	-5	
6 (P)P (3, 3,s)	2 A2' 1 s 2-1	nu24	2494.15364	0.1734E-02	0.1672E-02	3.60	-6	
7 (R)P (3, 0,s)	2 A2° 1 s 1 1	nu24	2482.17009	0.2148E-02	0.1654E-02	22.99	-2	
8 (R)R (1, 0,s)	2 A2'' 1 s 1 1	nu24	2581.51838	0.6725E-03	0.6344E-03	5.66	-1	
9 (R)P (3, 1,s)	2 E' 2 s 2 1	nu24	2474.84797	0.1585E-03	0.1496E-03	5.62	-2	
10 (R)R (1, 1,s)	2 E' 2 s 2 1	nu24	2574.21193	0.6521E-03	0.6186E-03	5.14	-2	
11 (P)P (3, 1,s)	2 E' 3 s 0 1	nu24	2486.86308	0.6954E-03	0.6607E-03	5.00	0	
12 (P)Q (2, 1,s)	2 E' 3 s 0 1	nu24	2546.46099	0.3333E-03	0.3164E-03	5.07	0	
13 (P)R (1, 1,s)	2 E' 3 s 0 1	nu24	2586.22677	0.3623E-04	0.3311E-04	8.62	0	
14 (P)P (3, 2,s)	2 E'' 2 s 1-1	nu24	2491.06980	0.8189E-03	0.7795E-03	4.81	-2	
15 (P)P (4, 3,s)	3 A2' 2 s 2-1	nu24	2476.51890	0.1771E-02	0.1707E-02	3.61	-1	
16 *(O)P (4, 3,s)	3 A2' 3 a 1 1	nu24	2542.60534	0.5772E-04	0.5119E-04	11.31	8	
17 (R)Q (3, 0,s)	3 A2° 2 s 1 1	nu24	2541.67426	0.2543E-02	0.2461E-02	3.21	4	
18 *(S)Q (3, 0,s)	3 A2° 3 a 2-1	nu24	2566.26140	0.1525E-03	0.1510E-03	1.01	0	
19 (R)P (4, 1,s)	3 E' 2 s 2 1	nu24	2456.98077	0.2308E-03	0.2226E-03	3.57	2	
20 (R)Q (3, 1,s)	3 E' 2 s 2 1	nu24	2536.35050	0.9171E-03	0.8738E-03	4.72	2	
21 (R)R (2, 1,s)	3 E' 2 s 2 1	nu24	2595.94834	0.3070E-03	0.2940E-03	4.22	2	
22 *(S)Q (3, 1,s)	3 E' 3 a 3-1	nu24	2547.13932	0.8439E-04	0.7592E-04	10.03	-1	
23 (P)P (4, 1,s)	3 E' 4 s 0 1	nu24	2469.37589	0.8114E-03	0.7827E-03	3.54	2	
24 (P)Q (3, 1,s)	3 E' 4 s 0 1	nu24	2548.74552	0.2544E-03	0.2429E-03	4.51	2	
25 (P)P (4, 4,s)	3 E'' 2 s 3-1	nu24	2478.45030	0.9730E-03	0.8368E-03	14.00	-6	
26 (R)P (4, 2,s)	3 E'' 3 s 3 1	nu24	2449.51292	0.1234E-03	0.1173E-03	4.98	-2	
27 (R)Q (3, 2,s)	3 E'' 3 s 3 1	nu24	2528.92016	0.7736E-03	0.7360E-03	4.86	-1	
28 (R)R (2, 2,s)	3 E'' 3 s 3 1	nu24	2588.54611	0.1062E-02	0.9988E-03	5.95	-2	
29 (P)P (4, 2,s)	3 E'' 4 s 1-1	nu24	2473.48104	0.8480E-03	0.8187E-03	3.45	1	
30 (P)Q (3, 2,s)	3 E'' 4 s 1-1	nu24	2552.88787	0.1519E-03	0.1421E-03	6.43	1	
31 (fJ)p (4, 2,s)	3 E'' 6 a 0 1	nu24	2523.67282	0.2226E-04	0.2114E-04	5.04	2	
32 (R)P (5, 3,s)	4 A2' 1 S 4 1	nu24	2423.77159	0.1733E-03	0.1702E-03	1.82	-1	
33 (R)Q (4, 3,s)	4 A2' 1 S 4 1	nu24	2522.95718	0.1505E-02	0.1473E-02	2.16	-1	
34 (R)R (3, 3,s)	4 A2' 1 S 4 1	nu24	2602.42682	0.2612E-02	0.2511E-02	3.85	-1	
35 (P)P (5, 3,s)	4 A2' 2 s 2-1	nu24	2459.68167	0.1609E-02	0.1545E-02	3.98	1	
36 (P)Q (4, 3,s)	4 A2' 2 s 2-1	nu24	2558.86726	0.7091E-04	0.7066E-04	0.36	1	
37 *(O)P (5, 3,s)	4 A2' 3 a 1 1	nu24	2519.51733	0.9588E-04	0.5679E-04	40.77	-10	
38 (R)P (5, 0,s)	4 A2'' 3 S1 1	nu24	2449.35160	0.1943E-02	0.1970E-02	-1.39	0	
39 (P)P (5, 5,s)	4 E' 3 s 4-1	nu24	2462.35303	0.8080E-03	0.7248E-03	10.30	-7	
40 (R)P (5, 1,s)	4 E' 4 s 2 1	nu24	2439.62165	0.1975E-03	0.1940E-03	1.75	4	
41 (R)Q (4, 1,s)	4 E' 4 s 2 1	nu24	2538.68380	0.8373E-03	0.8185E-03	2.25	5	
42 *(S)Q (4, 1,s)	4 E' 5 a 3-1	nu24	2548.81178	0.1729E-03	0.1628E-03	5.87	-1	
43 (P)Q (4, 1,s)	4 E' 6 s 0 1	nu24	"2551.87568	0.1348E-03	0.1342E-03	0.47	5	
44 *(Q)Q (4, 1,s)	4 E' 8 a 1-1	nu24	2586.35800	0.3979E-04	0.4880E-04	-22.65	3	
45 (P)P (5, 4,s)	4 E'' 2 s 3-1	nu24	2461.56809	0.8021E-03	0.7673E-03	4.34	0	
46 (S)p (5, 2,s)	4 E'' 3 a 4-1	nu24	2428.34322	0.2134E-04	0.2625E-04	-23.00	1	
47 (S)Q (4, 2,s)	4 E* 3 a 4-1	nu24	2527.45134	0.1135E-03	0.1125E-03	0.92	2	
48 (R)P (5, 2,s)	4 E'' 4 s 3 1	nu24	2433.75109	0.1585E-03	0.1529E-03	3.51	1	
49 (R)Q (4, 2,s)	4 E'' 4 s 3 1	nu24	2532.85931	0.8603E-03	0.8260E-03	3.99	1	
50 (R)R (3, 2,s)	4 E'' 4 s 3 1	nu24	2612.26634	0.4898E-03	0.4806E-03	1.87	1	
51 (P)P (5, 2,s)	4 E'' 5 s 1-1	nu24	2456.71733	0.7782E-03	0.7602E-03	2.31	2	
52 (P)Q (4, 2,s)	4 E'' 5 s 1-1	nu24	2555.82551	0.1042E-03	0.1040E-03	0.20	2	
53 (R)P (6, 3,s)	5 A2' 3 s 4 1	nu24	2408.28844	0.2478E-03	0.2420E-03	2.33	3	
54 (R)Q (5, 3,s)	5 A2' 3 s 4 1	nu24	2527.09025	0.1722E-02	0.1702E-02	1.17	3	
55 (R)R (4, 3,s)	5 A2' 3 s 4 1	nu24	2626.27578	0.1150E-02	0.1155E-02	-0.43	3	
56 (o)p (6, 3,s)	5 A2' 5 a 1 1	nu24	2508.35130	0.6226E-04	0.5285E-04	15.11	13	
57 (P)P (6, 6,s)	5 A2° 2 s 5-1	nu24	2445.86984	0.1181E-02	0.1124E-02	4.79	-9	
58 *(O)P (6, 6,s)	5 A2'' 3 a 4 1	nu24	2552.96526	0.5253E-04	0.5547E-04	-5.61	-2	
59 (R)Q (5, 0,s)	5 A2° 4 s 1 1	nu24	2545.72084	0.1564E-02	0.1573E-02	-0.57	8	
60 *(S)Q (5, 0,s)	5 A2° 5 a 2-1	nu24	2569.70851	0.2596E-03	0.2772E-03	-6.80	4	
61 (P)P (6, 5,s)	5 E' 3 s 4-1	nu24	2446.22530	0.6223E-03	0.6033E-03	3.06	0	
62 (R)P (6, 1,s)	5 E' 5 s 2 1	nu24	2422.67537	0.1167E-03	0.1215E-03	-4.10	4	
63 (R)Q (5, 1,s)	5 E' 5 s 2 1	nu24	2541.33152	0.6187E-03	0.6144E-03	0.70	4	
64 *(S)Q (5, 1,s)	5 E' 6 a 3-1	nu24	2550.98189	0.2212E-03	0.2130E-03	3.69	-1	
65 (P)P (6, 1,s)	5 E' 7 s 0 1	nu24	2437.22698	0.6886E-03	0.6883E-03	0.19	4	

Note.(I)Serial number;(II)Assignment;(III)Identification Of the upper level ;(IV)Vibrational band;(V)Observed wavenumber in CM-1; (VI)So in cm-2 atm-1 at 296K;(VII)Sc in cm-2 atm-1 at 296K;(VIII)So-Sc/So in %;(Obs-Calc)wavenumber in 10-3 cm-1

Table A.—Continued

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Intensity data from

(I)	Transit ion				(IV)	(V)	experiment	present	analysis	(IX)
	(II)	(III)					(VI)	(VII)	(VIII)	
66 (P)Q	5, 1,s)	5 E'	7 s o 1	nu24	2555.88310	0.4967E-04	0.5245E-04	-5.59	4	
67 *(O)P	6, 5,s)	5 E'	8 a 3 1	nu24	2536.67786	0.3838E-04	0.3193E-04	16.81	-1	
68 *(Q)Q	5, 1,s)	5 E"	9 a 1-1	nu24	2588.35971	0.4431E-04	0.5415E-04	-22.21	6	
69 (R)P	6, 4,s)	5 E"	3 5 5 1	nu24	2397.61607	0.6140E-04	0.5753E-04	6.30	-2	
70 (R)Q	5, 4,s)	5 E"	3 5 5 1	nu24	2516.54817	0.7439E-03	0.6661E-03	10.46	-1	
71 (R)R	4, 4,s)	5 E"	3 S 5 1	nu24	2615.84262	0.1403E-02	0.1359E-02	3.15	-2	
72 (P)P	6, 4,s)	5 E"	4 s 3-1	nu24	2445.46466	0.6401E-03	0.6175E-03	3.54	2	
73 *(S)Q	5, 2,s)	5 E"	5 a 4-1	nu24	2528.79288	0.7108E-04	0.7430E-04	-4.53	1	
74 (R)P	6, 2,s)	5 E"	6 S 3 1	nu24	2418.03181	0.1563E-03	0.1444E-03	7.61	5	
75 (R)Q	5, 2,s)	5 E"	6 S 3 1	nu24	2536.74236	0.8304E-03	0.7727E-03	6.95	5	
76 (R)R	4, 2,s)	5 E"	6 5 3 1	nu24	2635.85063	0.2080E-03	0.2297E-03	-10.42	5	
77 (P)P	6, 2,s)	5 E"	7 s 1-1	nu24	2440.80735	0.6282E-03	0.6244E-03	0.60	1	
78 (P)Q	5, 2,s)	5 E"	7 s 1-1	nu24	2559.51795	0.6256E-04	0.5601E-04	10.46	1	
79 (R)P	7, 3,s)	6 A2'	3 S 4 1	nu24	2393.34113	0.2206E-03	0.2095E-03	5.02	6	
80 (R)R	5, 3,s)	6 A2'	3 S 4 1	nu24	2650.44640	0.4321E-03	0.4533E-03	-4.90	6	
81 (P)P	7, 3,s)	6 A2'	4 s 2-1	nu24	2428.42338	0.8700E-03	0.8827E-03	-1.46	-1	
82 (P)Q	6, 3,s)	6 A2'	4 s 2-1	nu24	2566.72769	0.1644E-04	0.1474E-04	10.33	0	
83 (P)R	5, 3,s)	6 A2'	4 s 2-1	nu24	2685.52874	0.1456E-03	0.1408E-03	3.29	-1	
84 (P)P	7, 6,s)	6 A2°	2 s 5-1	nu24	2430.50325	0.8683E-03	0.8535E-03	1.70	2	
85 (P)Q	6, 6,s)	6 A2°	2 s 5-1	nu24	2569.38711	0.3748E-04	0.3706E-04	1.13	2	
86 (R)P	7, 0,s)	6 A2°	4 5 1 1	nu24	2420.23778	0.1019E-02	0.1075E-02	-5.53	-11	
87 (R)R	5, 0,s)	6 A2°	4 s 1 1	nu24	2676.98924	0.1180E-03	0.1216E-03	-3.05	-11	
88 (S)P	7, 0,s)	6 A2°	5 a 2-1	nu24	2434.11743	0.1570E-03	0.1181E-03	24.80	9	
89 (P)P	7, 7,s)	6 E'	3 S 6-1	nu24	2429.00825	0.4148E-03	0.3974E-03	4.20	-9	
90 (R)Q	6, 5,s)	6 E'	4 s 6 1	nu24	2509.68181	0.5748E-03	0.5504E-03	4.25	-2	
91 (R)R	5, 5,s)	6 E'	4 s 6 1	nu24	2628.78159	0.1344E-02	0.1313E-02	2.33	-2	
92 (P)P	7, 5,s)	6 E'	5 s 4-1	nu24	2430.85397	0.4471E-03	0.4374E-03	2.17	3	
93 (R)P	7, 1,s)	6 E'	7 S 2 1	nu24	2406.08912	0.5605E-04	0.5926E-04	-5.74	1	
94 *(S)Q	6, 1,s)	6 E'	8 a 3-1	nu24	2553.66660	0.2034E-03	0.2052E-03	-0.89	-3	
95 (P)P	7, 1,s)	6 E'	9 s o 1	nu24	2422.61904	0.5053E-03	0.5083E-03	-0.60	1	
96 (P)Q	6, 1,s)	6 E'	9 s o 1	nu24	2560.75129	0.1288E-04	0.1335E-04	-3.64	0	
97 *(O)P	7, 5,s)	6 E'	10 a 3	nu24	2518.02695	0.2784E-04	0.2515E-04	9.68	2	
98 (Q)Q	6, 1,s)	6 E'	11 a 1-	nu24	2590.95000	0.3902E-04	0.4871E-04	-24.83	6	
99 (R)P	7, 4,s)	6 E"	4 s 5	nu24	2382.98570	0.7834E-04	0.7629E-04	2.62	3	
100 (R)Q	6, 4,s)	6 E"	4 S 5	nu24	2521.43668	0.7268E-03	0.7045E-03	3.06	3	
101 (R)R	5, 4,s)	6 E"	4 s 5	nu24	2640.36825	0.5791E-03	0.5691E-03	1.73	3	
102 (P)P	7, 4,s)	6 E"	6 s 3-	nu24	2430.13444	0.4417E-03	0.4391E-03	0.58	1	
103 (S)Q	6, 2,s)	6 E"	7 a 4-	nu24	2530.74172	0.3323E-04	0.3780E-04	-13.76	0	
104 (R)P	7, 2,s)	6 E"	8 S 3	nu24	2402.68279	0.1067E-03	0.1016E-03	4.73	5	
105 (R)Q	6, 2,s)	6 E"	8 S 3	nu24	2540.87998	0.6087E-03	0.5921E-03	2.72	5	
106 (P)P	7, 2,s)	6 E"	9 s 1-	nu24	2425.77212	0.4564E-03	0.4534E-03	0.66	-1	
107 (P)Q	6, 2,s)	6 E"	9 S 1-	nu24	2563.96867	0.2115E-04	0.2189E-04	3.52	-2	
108 (O)P	7, 4,s)	6 E"	10 a 2	nu24	2500.49578	0.2352E-04	0.1852E-04	21.26	-1	
109 (R)Q	7, 3,s)	7 A2'	5 5 4	nu24	2536.51275	0.9038E-03	0.9206E-03	1.85	3	
110 (R)R	6, 3,s)	7 A2'	5 S 4	nu24	2674.81623	0.1241E-03	0.1470E-03	-18.46	3	
111 (P)P	8, 3,s)	7 A2'	6 s 2-	nu24	2413.95884	0.5464E-03	0.5563E-03	1.81	-3	
112 (P)R	6, 3,s)	7 A2'	6 S 2-	nu24	2709.92858	0.2210E-03	0.2033E-03	8.01	-3	
113 (R)Q	7, 6,s)	7 A2"	2 S 7	nu24	2502.34629	0.8746E-03	0.8364E-03	4.37	-3	
114 (R)R	6, 6,s)	7 A2°	2 s 7	nu24	2641.23000	0.2325E-02	0.2305E-02	0.86	-3	
115 (P)P	8, 6,s)	7 A2°	3 s 5-	nu24	2415.86210	0.5670E-03	0.5609E-03	1.08	4	
116 (P)Q	7, 6,s)	7 A2°	3 S 5-	nu24	2574.18369	0.4659E-04	0.4449E-04	4.51	4	
117 (P)R	6, 6,s)	7 A2"	3 S 5-	nu24	2713.06757	0.7809E-04	0.7480E-04	4.22	4	
118 (O)P	8, 6,s)	7 A2"	4 a 4	nu24	2515.99381	0.4253E-04	0.3983E-04	6.35	-2	
119 (R)Q	7, 0,s)	7 A2"	5 s 1	nu24	2551.19666	0.5893E-03	0.5957E-03	-1.09	2	
120 *(S)Q	7, 0,s)	7 A2"	6 a 2-	nu24	2575.28844	0.1604E-03	0.1998E-03	-24.55	4	
121 (P)P	8, 7,s)	7 E'	4 s 6-	nu24	2414.41325	0.2832E-03	0.2757E-03	2.64	4	
122 (R)Q	7, 5,s)	7 E'	5 s 6	nu24	2515.41770	0.5342E-03	0.5311E-03	0.57	3	
123 (R)R	6, 5,s)	7 E'	5 s 6 1	nu24	2654.06182	0.5100E-03	0.5036E-03	1.26	3	
124 (P)P	8, 5,s)	7 E'	6 s 4-1	nu24	2416.21954	0.2762E-03	0.2793E-03	-1.13	0	
125 (P)R	6, 5,s)	7 E'	6 s 4-1	nu24	2712.91630	0.7674E-04	0.7193E-04	6.27	0	
126 (R)Q	7, 1,s)	7 E'	8 S 2 1	nu24	2547.34084	0.2327E-03	0.2119E-03	8.94	-3	
127 *(S)Q	7, 1,s)	7 E'	9 a 3-1	nu24	2556.86352	0.1503E-03	0.1552E-03	-3.29	-6	
128 (P)P	8, 1,s)	7 E'	10 s o 1	nu24	2408.91587	0.3082E-03	0.3158E-03	-2.47	-5	
129 (P)R	6, 1,s)	7 E'	10 s o 1	nu24	2704.53024	0.9527E-04	0.8585E-04	9.89	-5	
130 (R)Q	7, 4,s)	7 E"	6 5 5	nu24	2526.73036	0.5185E-03	0.5177E-03	0.15	5	
131 (R)R	6, 4,s)	7 E"	6 s 5	nu24	2665.18126	0.1891E-03	0.2020E-03	-6.84	5	
132 (P)P	8, 4,s)	7 E"	8 s 3-	nu24	2415.56625	0.2712E-03	0.2773E-03	'2.26	-3	
133 (P)R	6, 4,s)	7 E"	8 S 3-	nu24	2711.85283	0.9608E-04	0.9313E-04	3.07	-2	
134 (R)Q	7, 2,s)	7 E"	10 S 3	nu24	2545.23882	0.3825E-03	0.3868E-03	-1.12	0	
135 (P)P	8, 2,s)	7 E"	11 s 1-	nu24	2411.61606	0.2800E-03	0.2906E-03	-3.80	-5	
136 (P)R	6, 2,s)	7 E"	11 S 1-	nu24	2707.36367	0.1011E-03	0.9874E-04	2.34	-5	

(I)	(II)	Transition					(VI)	(VII)	(VIII)	(IX)
		(111)	(IV)	(V)						
137	(R)Q (8, 3,s)	8 A2' 5 s 4 1	nu24	2541.59821	0.5160E-03	0.5294E-03	-2.60	-2		
138	(P)P (9, 3,s)	8 A2' 6 s 2-1	nu24	2400.38921	0.3064E-03	0.3160E-03	-3.13	-8		
139	(P)R (7, 3,s)	8 A2' 6 S 2-1	nu24	2734.94625	0.2251E-03	0.2188E-03	2.81	-8		
140	(R)Q (8, 6,s)	8 A2° 3 s 7 1	nu24	2508.98618	0.7388E-03	0.7361E-03	0.36	3		
141	(R)R (7, 6,s)	8 A2° 3 s 7 1	nu24	2667.30772	0.8079E-03	0.8116E-03	-0.46	3		
142	(P)P (9, 6,s)	8 A2° 4 s 5-1	nu24	2401.91367	0.3193E-03	0.3235E-03	-1.32	-1		
143	(P)Q (8, 6,s)	8 A2" 4 s 5-1	nu24	2579.51930	0.3692E-04	0.3692E-04	-0.01	-1		
144	(P)R (7, 6,s)	8 A2" 4 s 5-1	nu24	2737.84096	0.1380E-03	0.1365E-03	1.12	-1		
145	* (O)P (9, 6,s)	8 A2" 5 a 4 1	nu24	2497.75645	0.2878E-04	0.2240E-04	22.18	3		
146	(R)P (9, 0,s)	8 A2" 6 s 1 1	nu24	2394.30666	0.2756E-03	0.3087E-03	-12.02	-16		
147	(R)R (7, 0,s)	8 A2" 6 s 1 1	nu24	2728.41443	0.2636E-03	0.3187E-03	-20.90	-15		
148	* (S)P (9, 0,s)	8 A2° 7 a 2-1	nu24	2402.51428	0.1034E-03	0.8748E-04	15.40	-1		
149	(R)Q (8, 7,s)	8 E' 3 s 8 1	nu24	2494.52836	0.2976E-03	0.2936E-03	1.34	-4		
150	(R)R (7, 7,s)	8 E' 3 s 8 1	nu24	2653.17335	0.9597E-03	0.9290E-03	3.19	-4		
151	(P)P (9, 7,s)	8 E' 6 S 6-1	nu24	2400.50430	0.1651E-03	0.1647E-03	0.23	5		
152	(P)Q (8, 7,s)	8 E' 6 S 6-1	nu24	2578.46754	0.4600E-04	0.3250E-04	29.35	6		
153	(R)Q (8, 5,s)	8 E' 7 s 6	nu24	2521.50598	0.3467E-03	0.3545E-03	-2.25	4		
154	(R)R (7, 5,s)	8 E' 7 s 6	nu24	2679.55872	0.1601E-03	0.1638E-03	-2.30	5		
155	(P)P (9, 5,s)	8 E' 8 s 4-	nu24	2402.29586	0.1518E-03	0.1582E-03	-4.20	-5		
156	(P)R (7, 5,s)	8 E' 8 s 4-	nu24	2737.65766	0.1016E-03	0.9152E-04	9.92	-5		
157	● (0)P (9, 7,s)	8 E' 9 a 5	nu24	2513.78958	0.1623E-04	0.1436E-04	11.55	4		
158	● (S)Q (8, 1,s)	8 E' 11 a 3-	nu24	2560.56024	0.9101E-04	0.9566E-04	-5.11	-8		
159	(P)P (9, 1,9)	8 E' 13 s 0	nu24	2396.36677	0.1654E-03	0.1717E-03	-3.81	-6		
160	(P)R (7, 1,s)	8 E' 1 3 s 0	nu24	2730.52386	0.9999E-04	0.8813E-04	11.86	-6		
161	● (Q)Q (8,1,s)	8 E' 14 a 1-	nu24	2598.05702	0.1498E-04	0.2359E-04	-57.50	-2		
162	(P)P (9, 8,s)	8 E" 3 s 7-	nu24	2397.96606	0.1670E-03	0.1642E-03	1.69	8		
163	(P)Q (8, 8,s)	8 E" 3 s 7 -	nu24	2576.34839	0.4227E-04	0.3808E-04	9.90	9		
164	(R)Q (8, 4,s)	8 E" 8 s 5	nu24	2532.31075	0.3044E-03	0.3114E-03	-2.29	1		
165	(P)P (9, 4,s)	8 E" 9 s 3-	nu24	2401.73968	0.1475E-03	0.1560E-03	-5.78	-6		
166	(P)R (7, 4,s)	8 E" 9 s 3 -	nu24	2736.64497	0.1063E-03	0.1047E-03	1.50	-6		
167	(R)Q (8, 2,s)	8 E" 1 1 s 3	nu24	2549.75453	0.2073E-03	0.2199E-03	-6.06	-6		
168	(P)P (9, 2,S)	8 E" 12 s 1-	nu24	2398.31626	0.1510E-03	0.1643E-03	-8.83	-4		
169	(P)R (7, 2,S)	8 E" 12 s 1-	nu24	2732.62166	0.1102E-03	0.1121E-03	-1.76	-4		
170	(P)P (10, 9,s)	9 A2' 2 s 8-1	nu24	2381.17190	0.1817E-03	0.1812E-03	0.26	15		
171	(P)Q ("9, 9,s)	9 A2' 2 S 8-1	nu24	2579.26598	0.7471E-04	0.7166E-04	4.08	15		
172	(R)Q (9, 3,S)	9 A2' 6 s 4 1	nu24	2546.78074	0.2459E-03	0.2664E-03	-8.32	-9		
173	(P)P (10, 3,S)	9 A2' 7 s 2-1	nu24	2387.41984	0.1463E-03	0.1567E-03	-7.14	12		
174	(P)R (8, 3,S)	9 A2' 7 s 2-1	nu24	2760.23851	0.1783E-03	0.1986E-03	-11.39	12		
175	(R)R (8, 6,S)	9 A2° 4 s 7 1	nu24	2693.51500	0.2427E-03	0.2428E-03	-0.06	3		
176	(P)R (8, 6,S)	9 A2" 5 s 5-1	nu24	2762.94480	0.1456E-03	0.1503E-03	'3.25	-8		
177	● (S)Q (9, 0,S)	9 A2° 8 a 2-1	nu24	2583.32858	0.5328E-04	0.7363E-04	-38.19	0		
178	(R)Q (9, 7,s)	9 E' 5 s 8 1	nu24	2502.12416	0.2327E-03	0.2356E-03	-1.27	2		
179	(R)R (8, 7,s)	9 E' 5 's 8 1	nu24	2680.08634	0.3048E-03	0.3004E-03	1.43	1		
180	(P)R (8, 7,s)	9 E' 8 S 6-1	nu24	2762.30720	0.5533E-04	0.5569E-04	-0.65	-2		
181	(R)Q (9, s,s)	9 E' 9 s 6 1	nu24	2527.82311	0.1878E-03	0.1933E-03	-2.92	0		
182	(P)R (8, 5,S)	9 E' 10 s 4-1	nu24	2762.75437	0.8549E-04	0.8722E-04	-2.03	-6		
183	(R)Q (9, 1,s)	9 E' 1 2 s 2 1	nu24	2554.27104	0.4619E-04	0.4844E-04	-4.87	-3		
184	(P)P (10, 1,s)	9 E' 1 5 s 0 1	nu24	2384.23499	0.8653E-04	0.8829E-04	-2.03	-6		
185	(R)Q (9, 8,s)	9 E" 3 s 9 1	nu24	2486.21427	0.1891E-03	0.1911E-03	-1.08	-5		
186	(R)R (8, 8,s)	9 E" 3 s 9 1	nu24	2664.59635	0.7155E-03	0.6919E-03	3.30	-5		
187	(P)P (10, 8,s)	9 E" 6 s 7-1	nu24	2384.79567	0.8456E-04	0.8934E-04	-5.65	8		
188	(P)Q (9, 8 ,s)	9 E" 6 S 7-1	nu24	2582.36046	0.3807E-04	0.3358E-04	11.79	8		
189	(P)R (8, 8 ,s)	9 E" 6 S 7-1	nu24	2760.74298	0.2828E-04	0.2839E-04	-0.39	8		
190	(R)Q (9, 4 ,s)	9 E" 1 0 s 5 1	nu24	2538.06132	0.1528E-03	0.1611E-03	-5.45	-6		
191	(R)R (8, 4 ,s)	9 E" 1 0 s 5 1	nu24	2715.13251	0.1557E-04	0.1309E-04	15.90	-4		
192	(P)R (8, 4 ,s)	9 E" 12 s 3-1	nu24	2761.83065	0.8877E-04	0.9401E-04	-5.91	0		
193	(R)Q (9, 2 ,s)	9 E" 1 3 s 3 1	nu24	2554.37132	0.1026E-03	0.1102E-03	-7.39	-6		
194	(P)P (10, 2,s)	9 E" 14 s 1-1	nu24	2385.81754	0.7775E-04	0.8204E-04	'5.52	8		
195	(P)R (8, 2,s)	9 E" 14 s 1-1	nu24	2758.36849	0.9621E-04	0.1013E-03	-5.29	8		
196	(R)Q (10, 9,s)	10 A2' 1 s 10 1	nu24	2477.38898	0.2195E-03	0.2314E-03	-5.43	-4		
197	(R)R (9, 9,s)	10 A2' 1 s 10 1	nu24	2675.48310	0.9876E-03	0.9560E-03	3.20	-4		
198	(P)Q (10, 9,s)	10 A2' 3 s 8-1	nu24	2585.87805	0.5838E-04	0.5625E-04	3.65	13		
199	(P)R (9, 9,s)	10 A2' 3 S 8-1	nu24	2783.97217	0.4139E-04	0.4174E-04	-0.86	13		
200	(P)R (9, 3,s)	10 A2' 7 s 2-1	nu24	2786.10858	0.1329E-03	0.1419E-03	-6.79	12		
201	(R)Q (10, 6,s)	10 A2° 5 s 7 1	nu24	2522.98855	0.2113E-03	0.2216E-03	-4.86	-1		
202	(R)R (9, 6,s)	10 A2" 5 s 7 1	nu24	2719.70985	0.5293E-04	0.5966E-04	-12.71	0		
203	(P)R (9, 6,s)	10 A2° 6 S 5-1	nu24	2788.30236	0.1207E-03	0.1251E-03	-3.65	-6		
204	(R)Q (10, 7,s)	10 E' 7 s 8 1	nu24	2509.92081	0.1210E-03	0.1304E-03	-7.73	2		
205	(R)R (9, 7,s)	10 E' 7 s 8 1	nu24	2707.02974	0.7793E-04	0.8281E-04	-6.26	2		
206	(P)R (9, 7,s)	10 E' 10 s 6-1	nu24	2787.73551	0.5425E-04	0.5413E-04	0.22	-12		
207	(R)Q (10, 5,s)	10 E' 11 s 6 1	nu24	2534.24898	0.8831E-04	0.9064E-04	-2.64	-6		

Table X. Continued

(I)	Transition					Intensity data from				
	(II)		(III)		(IV)	(V)		experiment	present	analysis
	(VI)	(VII)	(VIII)	(IX)						
208 (P)R (9, 5,S) 10 E' 12 s 4-	nu24	2788.13228	0.6311E-04	0.6738E-04	-6.77	7				
209 (R)Q (10, 1,S) 10 E' 14 S 2	nu24	2558.03983	0.2004E-04	0.2105E0 4	-5.03	17				
210 (R)R (10, 9,S) 11 A2' 2 s10	nu24	2704.18581	0.2611E-03	0.2609E-03	0.09	-1				
211 (P)R (10, 6,s) 11 A2° 7 S 5	nu24	2813.82677	0.7241E-04	0.8495E-04	-17.31	18				
212 (R)Q (11, 5,s) 11 E' 1 2 s 6	nu24	2540.67194	0.3168E-04	0.3742E-04	-18.11	0				
213 (R)Q (11, 10,s) 11 E" 2 s11	nu24	2468.03783	0.6107E-04	0.6526E-04	-6.87	0				
214 (R)R (10, 10,s) 11 E" 2 s11	nu24	2685.81684	0.3151E-03	0.3073E-03	2.47	0				
215 (R)Q (12, 6,s) 12 A2" 7 s 7	nu24	2537.13580	0.2670E-04	0.3547E-04	'32.85	15				
216 (R)Q (12, 11,s) 12 E' 3 s12	nu24	2458.14430	0.3165E-04	0.3436E-04	-8.56	6				
217 (R)R (11, 11,s) 12 E' 3 s12 1	nu24	2695.58075	0.1919E-03	0.1843E-03	3.98	7				
218 (R)R (11, 10,s) 12 E" 4 SII 1	nu24	2715.48070	0.7865E-04	0.7700E-04	2.09	-5				
219 (R)Q (12, 8,s) 12 E" 9 s 9 1	nu24	2512.21683	0.2469E-04	0.2904E-04	'17.62	3				

Table XI

Comparison of Measured and Calculated Line Intensities in $v_2 + v_4$ a₁ -- a

(I)	Transition				Intensity data from				
	(II)		(III)		(IV)	(V)	experiment	present analysis	
	(VI)	(VII)	(VIII)	(IX)					
1 (R)P (2, 0,a)	1 A2'	2 a 1 1	nu24	2545.18036	0.1042E-02	0.9778E-03	6.16	-3	
2 (R)R (0, 0,a)	1 A2'	2 a 1 1	nu24	2604.79994	0.6961E-03	0.6679E-03	4.05	-3	
3 (P)P (2, 2,a)	1 E'	2 a 1-1	nu24	2553.78277	0.6534E-03	0.6155E-03	5.80	-4	
4 (P)Q (1, 1,a)	E"	3 a 0 1	nu24	2589.37002	0.2152E-03	0.2106E-03	2.12	-4	
5 *(S)Q (2, 0,a)	2 A2'	1 s 2-1	nu24	2519.60193	0.3430E-04	0.3209E-04	6.43	-6	
6 (R)Q (2, 0,a)	2 A2'	2 a 1 1	nu24	2584.42897	0.2269E-02	0.2246E-02	1.03	-10	
7 *(O)P (3, 3,a)	2 A2°	1 s 1 1	nu24	2514.75100	0.5260E-04	0.4709E-04	10.47	-1	
8 (P)P (3, 3,a)	2 A2°	2 a 2-1	nu24	2538.19432	0.1573E-02	0.1537E-02	2.27	-2	
9 (P)P (3, 2,a)	2 E'	4 a 1-1	nu24	2534.60094	0.8509E-03	0.8054E-03	5.34	-2	
10 (P)Q (2, 2,a)	2 E'	4 a 1-1	nu24	2594.19641	0.7072E-04	0.7166E-04	-1.33	-3	
11 (R)P (3, 1,a)	2 E"	3 a 2 1	nu24	2520.36253	0.1970E-03	0.1698E-03	13.79	-6	
12 (R)Q (2, 1,a)	2 E"	3 a 2 1	nu24	2579.93140	0.7401E-03	0.6867E-03	7.22	-6	
13 (R)R (1, 1,a)	2 E"	3 a 2 1	nu24	2619.67662	0.6106E-03	0.4994E-03	18.20	-7	
14 (P)P (3, 1,a)	2 E"	4 a O 1	nu24	2530.49695	0.8112E-03	0.7515E-03	7.36	-2	
15 (P)Q (2, 1,a)	2 E"	4 a O 1	nu24	2590.06609	0.2384E-03	0.2330E-03	2.27	-2	
16 *(S)P (4, 0,a)	3 A2'	2 s 2-1	nu24	2442.55596	0.4000E-04	0.2118E-04	47.04	-1	
17 (R)P (4, 0,a)	3 A2'	3 a 1 1	nu24	2508.64297	0.2496E-02	0.2524E-02	-1.13	8	
18 (P)P (4, 3,a)	3 A2°	3 a 2-1	nu24	2519.41160	0.1759E-02	0.1730E-02	1.63	0	
19 (o)p (4, 4,a)	3 E'	2 s 2 1	nu24	2511.72359	0.8182E-04	0.7394E-04	9.64	2	
20 (P)P (4, 4,a)	3 E'	3 a 3-1	nu24	2522.51248	0.7441E-03	0.7216E-03	3.02	-2	
21 (R)P (4, 2,a)	3 E'	5 a 3 1	nu24	2495.65006	0.1566E-03	0.1425E-03	9.02	-5	
22 (R)Q (3, 2,a)	3 E'	5 a 3 1	nu24	2575.01919	0.8565E-03	0.8077E-03	5.70	-5	
23 (R)R (2, 2,a)	3 E'	5 a 3 1	nu24	2634.61567	0.8412E-03	0.8176E-03	2.81	-5	
24 (P)P (4, 2,a)	3 E'	6 a 1-1	nu24	2515.86166	0.9513E-03	0.9200E-03	3.29	0	
25 (P)Q (3, 2,a)	3 E'	6 a 1-1	nu24	2595.23093	0.7026E-04	0.6625E-04	5.71	0	
26 (S)R (2, 1,a)	3 E"	2 s 3-1	nu24	2561.09872	0.1618E-04	0.1703E-04	5.24	-7	
27 *(Q)P (4, 1,a)	3 E"	4 s 1-1	nu24	2461.69792	0.2291E-04	0.1309E-04	42.88	0	
28 *(Q)Q (3, 1,a)	3 E"	4 s 1-1	nu24	2541.03160	0.2505E-04	0.2874E-04	--14.72	1	
29 (R)P (4, 1,a)	3 E"	5 a 2 1	nu24	2501.39645	0.2873E-03	0.2551E-03	11.22	-5	
30 (R)Q (3, 1,a)	3 E"	5 a 2 1	nu24	2580.72992	0.1003E-02	0.9648E-03	3.81	-5	
31 (R)R (2, 1,a)	3 E"	5 a 2 1	nu24	2640.29898	0.2122E-03	0.2057E-03	3.05	-5	
32 (P)Q (3, 1,a)	3 E"	6 a 0 1	nu24	2591.22319	0.1774E-03	0.1683E-03	5.15	1	
33 *(S)Q (4, 0,a)	4 A2'	2 s 2-1	nu24	2524.90422	0.1514E-03	0.1307E-03	13.6S	1	
34 (R)Q (4, 0,a)	4 A2'	3 a 1 1	nu24	2584.73917	0.2083E-02	0.2079E-02	0.21	-11	
35 (R)P (5, 3,a)	4 A2°	2 a 4 1	nu24	2470.71278	0.2359E-03	0.2127E-03	9.82	-4	
36 (R)Q (4, 3,a)	4 A2°	2 a 4 1	nu24	2569.85150	0.1793E-02	0.1688E-02	5.87	-4	
37 (R)R (3, 3,a)	4 A2°	2 a 4 1	nu24	2649.28162	0.2118E-02	0.2067E-02	2.41	-4	
38 (o)p (5, 3,a)	4 A2"	3 s 1 1	nu24	2481.76659	0.1621E-03	0.1305E-03	19.47	0	
39 (o)Q (4, 3,a)	4 A2"	3 s 1 1	nu24	2580.90489	0.3684E-04	0.5930E-04	-60.97	0	
40 (o)p (5, 4,a)	4 E'	4 s 2 1	nu24	2494.18198	0.1488E-03	0.1384E-03	6.97	5	
41 (P)P (5, 4,a)	4 E'	5 a 3-1	nu24	2504.30977	0.6930E-03	0.6852E-03	1.13	-1	
42 *(O)Q (4, 2,a)	4 E'	6 s 0 1	nu24	2562.22878	0.3651E-04	0.4364E-04	-19.53	4	
43 (R)P (5, 2,a)	4 E'	7 a 3 1	nu24	2477.09727	0.2241E-03	0.2153E-03	3.93	-3	
44 (R)Q (4, 2,a)	4 E'	7 a 3 1	nu24	2576.16095	0.1056E-02	0.1011E-02	4.26	-3	
45 (R)R (3, 2,a)	4 E'	7 a 3 1	nu24	2655.53027	0.3142E-03	0.3169E-03	-0.85	-3	
46 (P)P (5, 2,a)	4 E'	8 a 1-1	nu24	2497.64781	0.9168E-03	0.9161E-03	0.07	3	
47 (P)Q (4, 2,a)	4 E'	8 a 1-1	nu24	2596.71125	0.3483E-04	0.3517E-04	-0.99	3	
48 (P)P (5, 5,a)	4 E"	3 a 4-1	nu24	2505.19288	0.6966E-03	0.6517E-03	6.44	1	
49 *(O)P (5, 5,a)	4 E"	4 s 3 1	nu24	2510.60076	0.4236E-04	0.4437E-04	-4.73	1	
50 (Q)Q (4, 1,a)	4 E"	5 s 1-1	nu24	2544.04316	0.3948E-04	0.4166E-04	-5.51	2	
51 (R)P (5, 1,a)	4 E"	6 a 2 1	nu24	2482.58776	0.2421E-03	0.2217E-03	8.41	-5	
52 (R)Q (4, 1,a)	4 E"	6 a 2 1	nu24	2581.60661	0.1001E-02	0.9717E-03	2.92	-5	
53 (P)P (5, 1,a)	4 E"	7 a 0 1	nu24	2493.92851	0.1020E-02	0.1020E-02	0.02	6	
54 (P)Q (4, 1,a)	4 E"	7 a O 1	nu24	2592.94738	0.8343E-04	0.8237E-04	1.27	6	
55 (P)P (6, 6,a)	5 A2'	2 a 5-1	nu24	2489.49782	0.1122E-02	0.1083E-02	3.51	0	
56 (R)P (6, 0,a)	5 A2'	5 a 1 1	nu24	2474.78175	0.2042E-02	0.2151E-02	-5.31	13	
57 *(S)Q (5, 3,a)	5 A2°	2 s 5-1	nu24	2464.21760	0.2118E-04	0.1282E-04	39.47	-9	
58 *(S)R (4, 3,a)	5 A2°	2 s 5-1	nu24	2563.35644	0.6314E-04	0.6670E-04	-5.63	-8	
59 (R)P (6, 3,a)	5 A2°	3 a 4 1	nu24	2452.56184	0.2984E-03	0.2917E-03	2.25	-3	
60 (R)Q (5, 3,a)	5 A2°	3 a 4 1	nu24	2571.31274	0.2003E-02	0.1946E-02	2.85	-3	
61 (R)R (4, 3,a)	5 A2°	3 a 4 1	nu24	2670.45154	0.7350E-03	0.7358E-03	-0.11	-3	
62 *(O)P (6, 3,a)	5 A2"	4 s 1 1	nu24	2459.38490	0.1792E-03	0.1332E-03	25.65	7	
63 *(O)Q (5, 3,a)	5 A2°	4 s 1 1	nu24	2578.13576	0.3002E-04	0.5451E-04	-81.57	7	
64 (P)P (6, 3,a)	5 A2"	5 a 2-1	nu24	2483.37259	0.1389E-02	0.1431E-02	-3.03	4	

Note. (I) Serial number; (II) Assignment; (III) Identification of the upper level; (IV) Vibrational band; (V) Observed wavenumber in cm⁻¹; (VI) So in cm⁻² atm⁻¹ at 296K; (VII) Sc in cm⁻² atm⁻¹ at 296K; (VIII) So-Sc/So in %; (Obs-Calc) wavenumber in 10⁻³ cm⁻¹

Intensity data from

(I)	Transition				(IV)	(V)	-(VI)-	(VII)	(VIII)	(IX)
	(11)	(111)								
65 (P)R (4, 3,a)	5 A2"	5 a 2-1	nu24	2701.26229	0.2211E-03	0.2105E-03	4.81	4		
66 *(S)R (4, 2,a)	5 E'	3 s 4-1	nu24	2586.04102	0.3798E-04	0.4733E-04	24.62	0		
67 (R)P (6, 4,a)	5 E'	4 a 5 1	nu24	2445.55275	0.8715E-04	0.7476E-04	14.21	-3		
68 (R)Q (5, 4,a)	5 E'	4 a 5 1	nu24	2564.42885	0.8545E-03	0.7855E-03	8.07	-3		
69 (R)R (4, 4,a)	5 E'	4 a 5 1	nu24	2663.67408	0.1159E-02	0.1125E-02	2.97	-3		
70 *(O)P (6, 4,a)	5 E'	5 s 2 1	nu24	2477.01510	0.1946E-03	0.1727E-03	11.27	4		
71 (P)P (6, 4,a)	5 E'	6 a 3-1	nu24	2486.66548	0.5397E-03	0.5531E-03	-2.49	-1		
72 (P)R (4, 4,a)	5 E'	6 a 3-1	nu24	2704.78704	0.5708E-04	0.5787E-04	-1.38	-1		
73 (R)P (6, 2,a)	5 E'	8 a 3 1	nu24	2458.76970	0.1958E-03	0.1948E-03	0.50	-1		
74 (R)Q (5, 2,a)	5 E'	8 a 3 1	nu24	2577.43084	0.9137E-03	0.8870E-03	2.92	-1		
75 (P)P (6, 2,a)	5 E'	9 a 1-1	nu24	2480.05001	0.7803E-03	0.7959E-03	-1.99	6		
76 (P)Q (5, 2,a)	5 E'	9 a 1-1	nu24	2598.71111	0.1023E-04	0.9996E-05	2.29	6		
77 (P)R (4, 2,a)	5 E'	9 a 1-1	nu24	2697.77495	0.1199E-03	0.1161E-03	3.17	6		
78 *(S)Q (5, 1,a)	5 E"	4 s 3-	nu24	2508.41904	0.3648E-04	0.2718E-04	25.50	3		
79 (P)P (6, 5,a)	5 E"	5 a 4-	nu24	2486.60271	0.6519E-03	0.6242E-03	4.26	1		
80 *(Q)Q (5, 1,a)	5 E"	7 s 1-	nu24	2547.82497	0.4395E-04	0.4667E-04	-6.19	1		
81 (R)P (6, 1,a)	5 E"	8 a 2	nu24	2463.86515	0.1465E-03	0.1388E-03	5.24	-4		
82 (R)Q (5, 1,a)	5 E"	8 a 2	nu24	2582.47318	0.8179E-03	0.7977E-03	2.48	-4		
83 (P)P (6, 1,a)	5 E"	9 a 0	nu24	2476.71445	0.9393E-03	0.9156E-03	2.53	8		
84 (P)Q (5, 1,a)	5 E"	9 a 0	nu24	2595.32217	0.2714E-04	0.2621E-04	3.41	8		
85 (P)R (4, 1,a)	5 E"	9 a 0	nu24	2694.34133	0.1110E-03	0.1004E-03	9.58	9		
86 (P)P (7, 6,a)	6 A2'	2 a 5 -	nu24	2471.35556	0.9254E-03	0.9370E-03	-1.25	1		
87 (P)Q (6, 6,a)	6 A2'	2 a 5-1	nu24	2610.16832	0.1283E-03	0.1157E-03	9.83	1		
88 *(S)Q (6, 0,a)	6 A2'	4 s 2-1	nu24	2533.15761	0.1389E-03	0.1412E-03	-1.68	-1		
89 (R)Q (6, 0,a)	6 A2'	5 a 1 1	nu24	2585.29031	0.1041E-02	0.1062E-02	-2.04	-4		
90 *(S)R (5, 3,a)	6 A2"	2 s 5-1	nu24	2587.73435	0.7437E-04	0.1015E-03	-36.42	1		
91 (R)P (7, 3,a)	6 A2"	3 a 4 1	nu24	2434.67664	0.2562E-03	0.2533E-03	1.12	0		
92 (R)Q (6, 3,a)	6 A2°	3 a 4 1	nu24	2572.92193	0.1601E-02	0.1536E-02	4.03	0		
93 (R)R (5, 3,a)	6 A2°	3 a 4 1	nu24	2691.67292	0.1749E-03	0.1891E-03	-8.10	0		
94 *(O)P (7, 3,a)	6 A2°	4 s 1 1	nu24	2452.40793	0.1856E-03	0.1472E-03	20.70	-11		
95 (P)P (7, 3,a)	6 A2°	5 a 2-1	nu24	2466.28760	0.9775E-03	0.1029E-02	-5.25	9		
96 (P)R (5, 3,a)	6 A2°	5 a 2-1	nu24	2723.28400	0.3780E-03	0.3953E-03	-4.58	9		
97 *(S)R (5, 4,a)	6 E'	3 S 6-1	nu24	2563.84902	0.3122E-04	0.3423E-04	-9.64	-9		
98 *(S)Q (6, 2,a)	6 E'	5 s 4-1	nu24	2491.58983	0.2555E-04	0.1881E-04	26.40	3		
99 (R)P (7, 4,a)	6 E'	6 a 5 1	nu24	2427.83971	0.9933E-04	0.9773E-04	1.61	0		
100 (R)R (5, 4,a)	6 E'	6 a 5 1	nu24	2685.10773	0.3819E-03	0.3758E-03	1.59	0		
101 *(O)P (7, 4,a)	6 E'	7 s 2 1	nu24	2460.17155	0.1876E-03	0.1660E-03	11.50	1		
102 (P)P (7, 4,a)	6 E'	8 a 3-1	nu24	2469.61408	0.4434E-03	0.3889E-03	12.29	-4		
103 (P)R (5, 4,a)	6 E'	8 a 3-1	nu24	2726.88266	0.1264E-03	0.1402E-03	-10.92	-3		
104 *(O)P (7, 2,a)	6 E'	9 s 0 1	nu24	2432.95614	0.2690E-04	0.1695E-04	37.01	1		
105 *(O)Q (6, 2,a)	6 E'	9 s 0 1	nu24	2571.09986	0.3990E-04	0.5377E-04	-34.76	1		
106 (R)P (7, 2,a)	6 E'	10 a 3 1	nu24	2440.61814	0.1315E-03	0.1319E-03	-0.31	2		
107 (R)Q (6, 2,a)	6 E'	10 a 3 1	nu24	2578.76207	0.6349E-03	0.6313E-03	0.57	2		
108 (P)P (7, 2,a)	6 E'	11 a 1-1	nu24	2463.15303	0.6076E-03	0.6026E-03	0.82	6		
109 (P)R (5, 2,a)	6 E'	11 a 1-	nu24	2719.95780	0.2081E-03	0.2102E-03	-1.02	6		
110 (P)P (7, 7,a)	6 E"	3 a 6-	nu24	2473.05774	0.3903E-03	0.3793E-03	2.82	0		
111 (R)P (7, 5,a)	6 E"	5 a 6	nu24	2420.16619	0.5527E-04	0.4860E-04	12.06	-2		
112 (R)Q (6, 5,a)	6 E"	5 a 6	nu24	2558.74624	0.7282E-03	0.6647E-03	8.72	-1		
113 (R)R (5, 5,a)	6 E"	5 a 6	nu24	2677.78613	0.1112E-02	0.1091E-02	1.91	-1		
114 *(S)Q (6, 1,a)	6 E"	6 s 3-	nu24	2512.93178	0.3173E-04	0.2714E-04	14.46	1		
115 (P)P (7, 5,a)	6 E"	7 a 4-	nu24	2468.68214	0.5077E-03	0.4983E-03	1.85	0		
116 (P)R (5, 5,a)	6 E"	7 a 4-	nu24	2726.30177	0.5601E-04	0.4445E-04	20.64	0		
117 *(Q)Q (6, 1,a)	6 E"	9 s 1-	nu24	2552.37956	0.3507E-04	0.4256E-04	-21.37	-1		
118 (R)P (7, 1,a)	6 E"	10 a 2 1	nu24	2445.20990	0.6811E-04	0.6921E-04	-1.61	-2		
119 (R)Q (6, 1,a)	6 E"	10 a 2 1	nu24	2583.29251	0.5528E-03	0.5559E-03	-0.57	-2		
120 (P)P (7, 1,a)	6 E"	11 a 0 1	nu24	2460.29748	0.6571E-03	0.6941E-03	-5.63	8		
121 (P)R (5, 1,a)	6 E"	11 a 0 1	nu24	2716.98792	0.2145E-03	0.2110E-03	1.63	8		
122 (R)P (8, 6,a)	7 A2' 3 a 7 1	nu24	2394.55231	0.6158E-04	0.5879E-04	4.54	0			
123 (R)Q (7, 6,a)	7 A2'	3 a 7 1	nu24	2552.80048	0.1112E-02	0.1030E-02	7.36	0		
124 (R)R (6, 6,a)	7 A2'	3 a 7 1	nu24	2691.61322	0.1953E-02	0.1921E-02	1.63	0		
125 (P)P (8, 6,a)	7 A2'	4 a 5-1	nu24	2453.81966	0.6733E-03	0.6733E-03	0.01	0		
126 (P)Q (7, 6,a)	7 A2'	4 a 5-1	nu24	2612.06749	0.1396E-03	0.1266E-03	9.28	0		
127 (P)R (6, 6,a)	7 A2'	4 a 5-1	nu24	2750.88050	0.1343E-03	0.1200E-03	10.68	0		
128 (R)P (8, 3,a)	7 A2"	4 a 4 1	nu24	2416.93682	0.1361E-03	0.1475E-03	-8.37	-2		
129 (R)Q (7, 3,a)	7 A2"	4 a 4 1	nu24	2574.55065	0.9982E-03	0.1023E-02	-2.45	-2		
130 (R)R (6, 3,a)	7 A2"	4 a 4 1	nu24	2712.79606	0.2160E-04	0.2239E-04	-3.65	-2		
131 (P)R (6, 3,a)	7 A2°	6 a 2-	nu24	2745.70410	0.4738E-03	0.5116E-03	-7.98	4		
132 (P)P (8, 8,a)	7 E'	3 a 7 -	nu24	2456.35719	0.2551E-03	0.2449E-03	4.01	-2		
133 (R)P (8, 4,a)	7 E'	7 a 5	nu24	2410.39686	0.7656E-04	0.7671E-04	-0.19	1		
134 (R)Q (7, 4,a)	7 E'	7 a 5	nu24	2568.17105	0.6040E-03	0.5897E-03	2.36	1		
135 (R)R (6, 4,a)	7 E'	7 a 5	nu24	2706.56265	0.8676E-04	0.9156E-04	-5.53	1		

Table XI_Continued

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Intensity data from

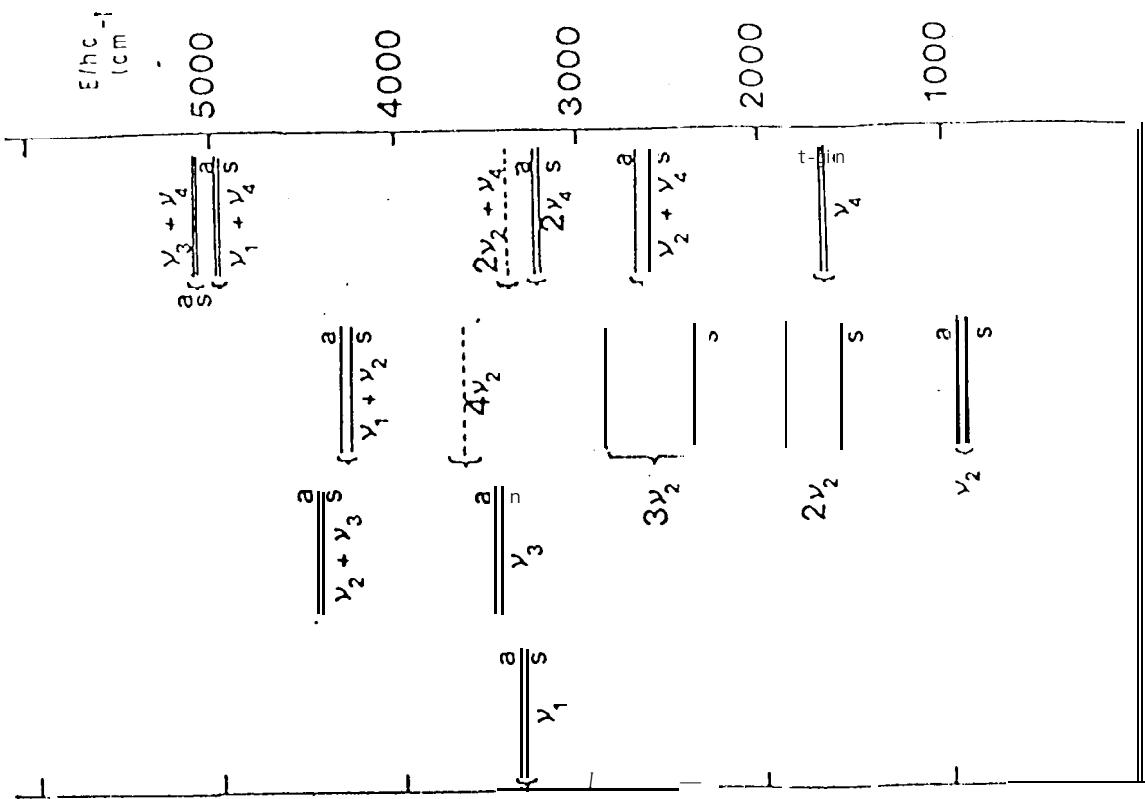
(I)	Transition			(xv)	(v)	(VI)	experiment	present	analysis	(IX)
	(I I)	(111) --	(VII)				(VII)	(v III)		
136	(P)P (8 , 4,a)	7 E' 9 a 3-1	nu24	2453.17173	0.2304E-03	0.2437E-03	-5.77	-7		
137	(P)R (6 , 4,a)	7 E' 9 a 3-1	nu24	2749.33747	0.1689E-03	0.1997E-03	-18.25	-7		
138	(O)Q (7 , 2,a)	7 E' 10 s 0 1	nu24	2576.73268	0.5326E-04	0.6446E-04	-21.03	-5		
139	(R)P (8 , 2,a)	7 E' 11 a 3 1	nu24	2422.63996	0.7289E-04	0.7533E-04	-3.35	8		
140	(R)Q (7 , 2,a)	7 E' 11 a 3 1	nu24	2580.13486	0.3610E-03	0.3635E-03	-0.68	7		
141	(P)P (8 , 2,a)	7 E' 12 a 1-	nu24	2447.01840	0.3701E-03	0.3976E-03	-7.43	3		
142	*(S)R (6 , 5,a)	7 E" 3 s 7-	nu24	2563.91170	0.3513E-04	0.3049E-04	13.21	-9		
143	(P)P (8 , 7,a)	7 E" 5 a 6-	nu24	2455.30498	0.3054E-03	0.3016E-03	1.25	1		
144	(R)P (8 , 5,a)	7 E" 7 a 6	nu24	2402.90255	0.5524E-04	0.5858E-04	-6.05	0		
145	(R)Q (7 , 5,a)	7 E" 7 a 6	nu24	2560.88873	0.6664E-03	0.6309E-03	5.32	0		
146	(R)R (6 , 5,a)	7 E" 7 a 6	nu24	2699.46860	0.3366E-03	0.3390E-03	-0.70	0		
147	(P)P (8 , 5,a)	7 E" 9 a 4-	nu24	2451.40651	0.3424E-03	0.3414E-03	0.28	-2		
148	(P)R (6 , 5,a)	7 E" 9 a 4-	nu24	2747.97229	0.1105E-03	0.9367E-04	15.23	-1		
149	(R)P (8 , 1,a)	7 E" 12 a 2 1	nu24	2426.64664	0.2922E-04	0.2935E-04	-0.43	0		
150	(R)Q (7 , 1,a)	7 E" 12 a 2 1	nu24	2584.07284	0.3332E-03	0.3373E-03	-1.24	0		
151	(P)P (8 , 1,a)	7 E" 13 a 0 1	nu24	2444.67913	0.4208E-03	0.4502E-03	-6.99	3		
152	(P)R (6 , 1,a)	7 E" 13 a 0 1	nu24	2740.18814	0.2752E-03	0.2875E-03	-4.45	3		
153	(R)Q (8 , 6,a)	8 A2' 3 a 7 1	nu24	2555.28780	0.9197E-03	0.8918E-03	3.03	0		
154	(R)R (7 , 6,a)	8 A2' 3 a 7 1	nu24	2713.53582	0.5484E-03	0.5542E-03	-1.06	0		
155	(P)P (9 , 6,a)	8 A2' 4 a 5-1	nu24	2436.93196	0.4028E-03	0.4151E-03	-3.05	-1		
156	(P)R (7 , 6,a)	8 A2' 4 a 5-1	nu24	2772.71153	0.2306E-03	0.2135E-03	7.40	-1		
157	(R)Q (8 , 0,*)	8 A2' 7 a 1 1	nu24	2586.14900	0.3229E-03	0.3413E-03	-5.70	-1		
158	(R)P (9 , 3,a)	8 A2" 5 a 4 1	nu24	2399.48354	0.8218E-04	0.8124E-04	1.14	3		
159	(R)Q (8 , 3,a)	8 A2° 5 a 4 1	nu24	2576.30455	0.6384E-03	0.5576E-03	12.65	3		
160	(P)P (9 , 3a)	8 A2" 7 a 2-1	nu24	2434.35669	0.3100E-03	0.3459E-03	-11.57	-1		
161	(P)R (7 , 3,a)	8 A2° 7 a 2-1	nu24	2768.79224	0.4368E-03	0.5341E-03	-22.27	-1		
162	(P)P (9 , 8,a)	8 E' 5 a 7-1	nu24	2438.96074	0.1828E-03	0.1789E-03	2.11	1		
163	(R)P (9 , 4,a)	8 E' 9 a 5 1	nu24	2393.18796	0.4320E-04	0.4506E-04	-4.31	4		
164	(R)Q (8 , 4,a)	8 E' 9 a 5	nu24	2570.19555	0.3397E-03	0.3471E-03	-2.17	4		
165	(R)R (7 , 4,a)	8 E' 9 a 5	nu24	2727.97007	0.1179E-04	0.1246E-04	-5.68	4		
166	(o)P (9 , 4,a)	8 E' 1 0 s 2	nu24	2427.47224	0.9012E-04	0.8011E-04	11.11	-6		
167	(P)P (9 , 4,a)	8 E' 11 a 3-	nu24	2437.34046	0.1226E-03	0.1388E-03	-13.18	-9		
168	(P)R (7 , 4,a)	8 E' 11 a 3-	nu24	2772.12238	0.1728E-03	0.2123E-03	-22.86	-8		
169	(R)Q (8 , 2,a)	8 E' 1 2 a 3	nu24	2581.19823	0.2265E-03	0.2338E-03	-3.22	7		
170	(P)P (9 , 2,a)	8 E' 14 a 1-	nu24	2431.67903	0.2038E-03	0.2292E-03	-12.45	-2		
171	(P)R (7 , 2,a)	8 E' 14 a 1-	nu24	2765.87401	0.2478E-03	0.2808E-03	-13.30	-2		
172	(S)R (7 , 5,a)	8 E" 3 s 7-	nu24	2589.90464	0.3426E-04	0.3699E-04	-7.96	8		
173	(R)Q (8 , 7,a)	8 E" 5 a 8 1	nu24	2546.58859	0.4104E-03	0.3677E-03	10.40	1		
174	(R)R (7 , 7,a)	8 E" 5 a 8 1	nu24	2705.15086	0.8232E-03	0.7762E-03	5.71	1		
175	(P)P (9 , 7,a)	8 E" 6 a 6-1	nu24	2438.16523	0.2176E-03	0.1976E-03	9.19	0		
176	(P)R (7 , 7,a)	8 E" 6 a 6-1	nu24	2774.60715	0.5807E-04	0.5555E-04	4.34	0		
177	(R)P (9 , 5,a)	8 E" 7 a 6 1	nu24	2385.92728	0.4219E-04	0.4251E-04	-0.76	1		
178	(R)Q (8 , 5,a)	8 E" 7 a 6 1	nu24	2563.16970	0.4138E-03	0.4130E-03	0.18	2		
179	(R)R (7 , 5,a)	8 E" 7 a 6 1	nu24	2721.15524	0.7813E-04	0.7840E-04	-0.35	2		
180	(S)Q (8 , 1,a)	8 E" 9 s 3-1	nu24	2523.93404	0.1648E-04	0.1491E-04	9.56	-5		
181	(P)P (9 , 5,a)	8 E" 10 a 4-1	nu24	2434.79200	0.2031E-03	0.2038E-03	-0.32	-4		
182	(P)R (7 , 5,a)	8 E" 10 a 4-1	nu24	2770.01983	0.1359E-03	0.1185E-03	12.83	-4		
183	(R)Q (8 , 1,a)	8 E" 13 a 2 1	nu24	2584.84343	0.1676E-03	0.1814E-03	-8.21	0		
184	(P)P (9 , 1,a)	8 E" 14 a 0 1	nu24	2429.83767	0.2882E-03	0.2535E-03	12.05	-3		
185	(P)R (7 , 1,a)	8 E" 14 a 0 1	nu24	2763.88764	0.2761E-03	0.2940E-03	-6.50	-2		
186	*(S)R (8 , 6,a)	9 A2' 2 s 8-1	nu24	2590.38155	0.5009E-04	0.5246E-04	-4.74	15		
187	(R)Q (9 , 6a)	9 A2' 4 a 7	nu24	2557.91463	0.5362E-03	0.5314E-03	0.89	2		
188	(R)R (8 , 6,a)	9 A2' 4 a 7	nu24	2735.44629	0.1245E-03	0.1210E-03	2.79	2		
189	(P)P (10 , 6,a)	9 A2' 5 a 5 -	nu24	2420.72992	0.2089E-03	0.2232E-03	-6.86	-4		
190	(P)R (8 , 6,a)	9 A2' 5 a 5 -	nu24	2794.90999	0.2364E-03	0.2318E-03	1.93	-4		
191	(R)P (10 , 0,a)	9 A2' 9 a 1	nu24	2415.22066	0.2209E-03	0.2585E-03	-17.01	-6		
192	(R)R (8 , 0,a)	9 A2' 9 a 1	nu24	2787.44865	0.4244E-03	0.4925E-03	-16.04	-6		
193	(P)Q (9 , 9,a)	9 A2° 3 a 8-	nu24	2620.37695	0.1583E-03	0.1478E-03	6.62	2		
194	(R)P (10 , 3,a)	9 A2° 6 a 4	nu24	2381.97749	0.2454E-04	0.2976E-04	-21.28	0		
195	(R)Q (9 , 3,a)	9 A2° 6 a 4	nu24	2577.86955	0.2564E-03	0.2854E-03	-11.32	0		
196	(O)P (10 , 3,a)	9 A2° 7 s 1 1	nu24	2393.69013	0.4157E-04	0.3059E-04	26.42	8		
197	(P)P (10 , 3,a)	9 A2° 8 a 2-1	nu24	2419.27928	0.1739E-03	0.2081E-03	-19.69	0		
198	(P)R (8 , 3,a)	9 A2° 8 a 2-1	nu24	2791.99264	0.3716E-03	0.4449E-03	-19.72	0		
199	(R)Q (9 , 8,a)	9 E' 4 a 9 1	nu24	2540.10878	0.2662E-03	0.2429E-03	8.77	3		
200	(R)R (8 , 8,a)	9 E' 4 a 9 1	nu24	2718.39578	0.6081E-03	0.5791E-03	4.77	3		
201	(P)R (8 , 8,a)	9 E' 7 a 7-1	nu24	2797.95844	0.4767E-04	0.4446E-04	6.73			
202	(R)Q (9 , 4,a)	9 E' 11 a 5 1	nu24	2572.26120	0.1606E-03	0.1755E-03	-9.28	6		
203	(O)P (10 , 4,a)	9 E' 12 S 2 1	nu24	2411.65096	0.5053E-04	0.4133E-04	18.21	-4		
204	(P)P (10 , 4,a)	9 E' 13 a 3-1	nu24	2422.12856	0.6332E-04	0.7248E-04	-14.47	-2		
205	(P)R (8 , 4,a)	9 E' 13 a 3-1	nu24	2795.21475	0.1908E-03	0.1836E-03	3.76	-1		
206	(R)Q (9 , 2,a)	9 E' 14 a 3 1	nu24	2582.59362	0.9738E-04	0.1081E-03	-11.04	7		

Table XI_Continued

(I)	Transition					Intensity data from						
	(1 1)		(1 1 1)		(I v)	(V)	experiment	present	analysis	(IX)		
	(P)P	(10, 2,a)	9	E'	16	a 1-1	nu24	2417.13923	0.1024E-03	0.1160E-03	-13.23	-8
207	(P)R	(8, 2,a)	9	E'	16	a 1-1	nu24	2789.58004	0.2004E-03	0.2338E-03	-16.67	-8
208	(R)Q	(9, 7,a)	9	E"	7	a 8 1	nu24	2549.42554	0.2968E-03	0.2904E-03	2.16	-2
209	(R)R	(8, 7,a)	9	E"	7	a 8 1	nu24	2727.30449	0.2018E-03	0.2075E-03	-2.84	-2
210	(P)P	(10, 7,a)	9	E"	8	a 6-1	nu24	2421.68612	0.1049E-03	0.1106E-03	-5.43	-1
211	(P)R	(8, 7,a)	9	E"	8	a 6-1	nu24	2796.59217	0.9014E-04	0.8773E-04	2.67	-1
212	(R)Q	(9, 5,a)	9	E"	9	a 6 1	nu24	2565.54406	0.2152E-03	0.2205E-03	-2.45	6
213	(P)P	(10, 5,a)	9	E"	11	a 4-1	nu24	2418.85822	0.1026E-03	0.1067E-03	-3.96	-5
214	(P)R	(8, 5,a)	9	E"	11	a 4-1	nu24	2792.43303	0.1240E-03	0.1116E-03	10.03	-5
215	(S)Q	(9, 1,a)	9	E"	12	s 3-1	nu24	2530.32977	0.1465E-04	0.8679E-05	40.76	-2
216	(P)P	(10, 1,a)	9	E"	16	a 0 1	nu24	2415.74768	0.1082E-03	0.1254E-03	-15.87	-6
217	(P)R	(8, 1,a)	9	E"	16	a 0 1	nu24	2788.02884	0.2097E-03	0.2421E-03	-15.45	-6
218	(R)R	(9, 6,a)	10	A2'	4	a 7 1	nu24	2757.28845	0.1530E-04	0.1652E-04	-7.98	7
219	(P)P	(11, 6,a)	10	A2'	5	a 5-1	nu24	2405.24319	0.1032E-03	0.1057E-03	2.45	-4
220	(P)R	(9, 6,a)	10	A2'	5	a 5-1	nu24	2817.47651	0.1907E-03	0.1908E-03	-0.05	-3
221	(R)Q	(10, 9,a)	10	A2"	2	a 10 1	nu24	2533.35940	0.3225E-03	0.2977E-03	7.68	5
222	(R)R	(9, 9,a)	10	A2°	2	a 10 1	nu24	2731.34447	0.8342E-03	0.8013E-03	3.95	5
223	(P)P	(11, 9,a)	10	A2"	4	a 8-1	nu24	2406.00036	0.1013E-03	0.1075E-03	6.15	3
224	(P)Q	(10, 9,a)	10	A2"	4	a 8-1	nu24	2623.02384	0.1135E-03	0.1157E-03	-1.91	3
225	(P)R	(9, 9,a)	10	A2"	4	a 8-1	nu24	2821.00865	0.6804E-04	0.6399E-04	5.95	3
226	(P)P	(n, 10,a)	10	E'	4	a 9-1	nu24	2405.62268	0.5463E-04	0.5048E-04	7.60	5
227	(R)R	(9, 8,a)	10	E'	6	a 9 1	nu24	2740.76935	0.1407E-03	0.1433E-03	-1.86	-6
228	(P)P	(11, 8,a)	10	E'	9	a 7-1	nu24	2406.11643	0.4876E-04	0.5442E-04	-11.60	0
229	(P)R	(9, 8,a)	10	E'	9	a 7-1	nu24	2820.05821	0.6806E-04	0.6280E-04	7.73	0
230	(O)P	(11, 4,a)	10	E'	14	S 2 1	nu24	2396.16189	0.1782E-04	0.1769E-04	0.70	18
231	(O)R	(9, 4,a)	10	E'	14	5 2 1	nu24	2807.20846	0.2078E-04	0.8638E-05	58.43	17
232	(P)R	(9, 2,a)	10	E'	18	a 1-1	nu24	2813.73166	0.1379E-03	0.1634E-03	-18.48	-10
233	(R)Q	(10, 7,a)	10	E"	8	a 8 1	nu24	2552.40231	0.1503E-03	0.1577E-03	-4.94	0
234	(R)R	(9, 7,a)	10	E"	8	a 8 1	nu24	2749.42921	0.3850E-04	0.4261E-04	-10.67	0
235	(P)R	(9, 1,a)	10	EM	18	a 0 1	nu24	2812.55591	0.1368E-03	0.1668E-03	-21.95	-6
236	(P)P	(12, 6,a)	11	A2'	7	a 5-1	nu24	2390.48468	0.3884E-04	0.4433E-04	-14.13	0
237	(P)R	(10, 6,a)	11	A2'	7	a 5-1	nu24	2840.39631	0.1160E-03	0.1279E-03	-10.29	0
238	(R)Q	(11, 9,a)	11	A2"	3	a 10 1	nu24	2536.90191	0.1982E-03	0.1958E-03	1.21	-13
239	(R)R	(10, 9,a)	11	A2"	3	a 10 1	nu24	2753.92516	0.1819E-03	0.1833E-03	-0.78	-13
240	(R)Q	(11, 10,a)	11	E'	4	a 11 1	nu24	2526.33994	0.8841E-04	0.8491E-04	3.95	9
241	(R)R	(10, 10,a)	11	E'	4	a 11 1	nu24	2743.99514	0.2733E-03	0.2578E-03	5.66	9
242	(P)R	(10, 2,a)	11	E'	20	a 1-1	nu24	2838.27530	0.7298E-04	0.9773E-04	-33.92	-5
243	(P)R	(10, 1,a)	11	E"	20	a 0 1	nu24	2837.41561	0.7814E-04	0.9855E-04	-26.12	-1
244	(R)R	(11, 10,a)	12	E'	6	a 11 1	nu24	2766.76767	0.5316E-04	0.5447E-04	-2.47	-22
245	(R)Q	(12, 11,a)	12	E"	3	a 12 1	nu24	2519.05033	0.5295E-04	0.4516E-04	14.71	15
246	(R)R	(n, 11,a)	12	E"	3	a 12 1	nu24	2756.34631	0.1649E-03	0.1547E-03	6.18	15

(I) Transitions with $s > 0.1\text{-}0.006 \text{ cm}^{-2}\text{atm}^{-1}$ at 296K . (II) Identifications of the upper levels. (III) Vibrational band. (IV) Wavenumbers observed, or calculated for the lower levels. (V) (Obs-Calc) deviations in 10^{-4} cm^{-1} . (VI) Line strengths in cm^{-2} atm $^{-1}$ at 296K . (VII) Calculated upper state energies in cm^{-1} . (VIII) Calculated lower energies in cm^{-1} . (IX) Statistical weights used in the fit of the parameters.

(I)	(II)	(III)	(IV)	(V)	(VI)	(VII)	(VIII)	(IX)
Line positions and intensities in the system N_2/NH_3 of (14) NH_3 . (small portion)								
$**(-)\text{R}(12,\text{E},10,\text{a})$	13 3 Ee	8 s4 O Δ nu2 22887.67987	0.1863.00147	1175.32160	0.0			
$(\text{R})\text{R}(12,\text{A}^+,0,\text{a})$	13 A+ Δ e 13 e 7 1 nu2 2887.80705	228.4	0.293E-04	4420.01068	1532.22647	1.0		
$(\text{P})\text{R}(12,\text{E},7,\text{a})$	13 3 Eo	15 a 6-1 nu2 22887.89153	0.131E-04	4247.22038	1359.32885	0.0		
$(\text{P})\text{R}(12,\text{E},1,\text{a})$	13 3 Eo	25 e 0 1 nu2 22887.90157	0.146E-04	4416.63624	1528.73467	0.0		
$(\text{P})\text{R}(12,\text{E},1,\text{a})$	13 3 Eo	25 e 0 1 nu2 22887.90157	0.146E-04	4416.63624	1528.73467	0.0		
$(\text{O})\text{o}(4,\text{A}^+,3,\text{s})$	4 A- Δ e	4 a 3 O Δ nu2 2887.90672	-19.4	0.305E-02	3053.29374	165.33	108.1.0	
$(\text{P})\text{R}(12,\text{E},8,\text{a})$	13 3 Ee	14 e 7-1 nu2 22888.27182	0.131E-04	4193.92064	1305.64882	0.0		
$(\text{P})\text{R}(12,\text{E},2,\text{a})$	13 3 Ee	24 e 7 - 7 nu2 22888.28235	0.145 E-04	4406.53261	1518.25026	0.0		
$(\text{P})\text{R}(12,\text{A}^+,12,\text{a})$	13 A+ Δ e	3 11-1 nu2 22888.45924	0.2s-2E-06	4132.83102	1244.37178	0.0		
$(\text{P})\text{R}(12,\text{A}^-,9,\text{a})$	13 A- Δ e	6 - 8 - 1 nu2 22888.45924	0.131E-04	4193.92064	1305.64882	0.0		
$(\text{P})\text{R}(12,\text{A}^+,12,\text{a})$	13 3 Eo	8 110-1 nu2 22888.52217	0.960E-05	3901.57035	1013.05 460 0.0			
$(\text{P})\text{R}(12,\text{E},11,\text{a})$	13 3 Eo	9 e 9-1 nu2 22888.53905	0.111E-04	4063.86065	1175.32160	0.0		
$(\text{P})\text{R}(12,\text{E},10,\text{a})$	13 3 Ee	9 e 9-1 nu2 22888.53905	0.111E-04	4063.86065	1175.32160	0.0		
$(\text{P})\text{R}(11,\text{E},4,\text{a})$	12 E Ee	21 s 0 7 nu2 22889.04148	0.102E-06	4131.54653	1242.50505	0.0		
$(\text{P})\text{R}(11,\text{A}^-,6,\text{a})$	12 A- Δ e	8 s 4 1 nu2 22891.30233	0.749E-05	4062.53765	1171.23532	0.0		
$(\text{M})\text{R}(8,\text{A}^-,6,\text{s})$	9 A- Δ Zo	8 a 6 0 Δ nu2 2893.48263699. S	0.106E-05	3471.82898	880.77963	0.0		
$(\text{M})\text{R}(10,\text{A}^-,6,\text{s})$	10 A- Δ Zo	8 a 5 0 Δ nu2 2893.48263699. S	0.85E-03	3098.78590	205.26910	1.0		
$(\text{O})\text{o}(4,\text{E},4,\text{s})$	4 E Eo	8 e 4 O Δ nu2 2893.6112623	0.309E-02	3267.827745	283.57435	1.0		
$(\text{O})\text{o}(4,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.48263699. S	0.474E-02	3177.05033	283.57435	1.0		
$(\text{O})\text{o}(5,\text{S}^-,\text{5},\text{s})$	5 E Ee	10 e 5 Δ nu2 2893.4765167. 1	0.828E-03	3098.78590	205.26910	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.4765167. 1	0.180E-02	3267.827745	283.57435	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text{s})$	7 E Ee	13 a 7 O Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{A}^-,6,\text{s})$	6 A+ Δ Zo	6 a 6 0 Δ nu2 2893.6112623	0.309E-02	3032.96310	1339.35801	1.0		
$(\text{O})\text{o}(5,\text{E}^-,\text{5},\text$								



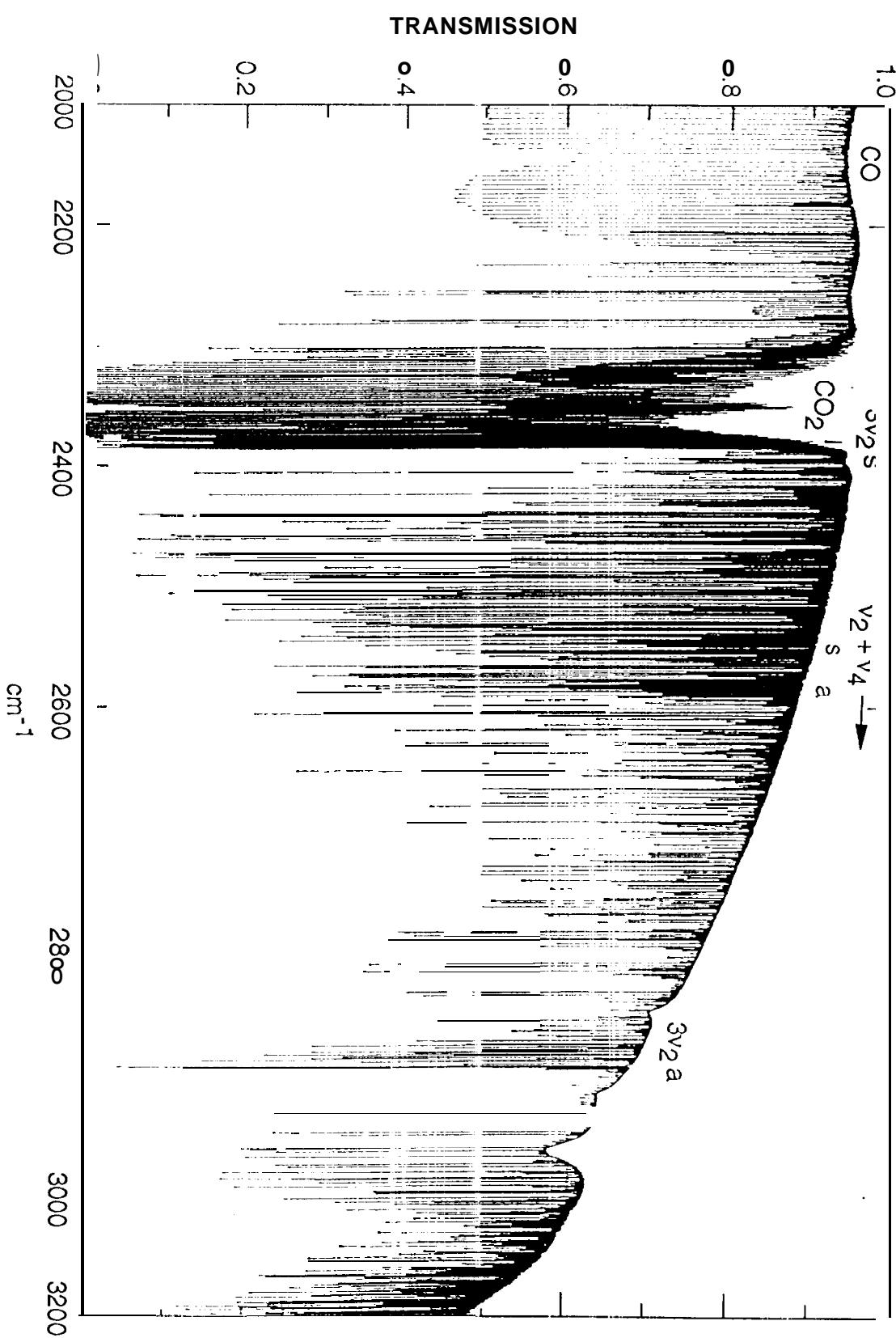


Fig. 3. Interaction Blocks in the Upper State Energy Matrix

$v_2 = 3; s$

$v_2 = 3; a$

$v_2 = v_4 = 1; s$

$v_2 = v_4 = 1; a$

Diagonal Terms. $\Delta K = \pm 6.$	$\Delta K = \pm 3.$	$\Delta v_2 = -2, \Delta v_4 = +1;$ $\Delta K = \pm 2, \Delta l_4 = \mp 1.$	$\Delta v_2 = -2, \Delta v_4 = +1;$ $\Delta K = \pm 1, \Delta l_4 = \pm 1.$
	Diagonal Terms. $\Delta K = \pm 6.$	$\Delta v_2 = -2, \Delta v_4 = +1;$ $\Delta K = \pm 1, \Delta l_4 = \pm 1.$	$\Delta v_2 = -2, \Delta v_4 = +1;$ $\Delta K = \pm 2, \Delta l_4 = \mp 1.$
		Diagonal Terms. $\Delta K = \pm 6.$ $\Delta K = \pm 2, \Delta l_4 = \pm 2.$ $\Delta K = \pm 4, \Delta l_4 = \mp 2.$	$\Delta K = \pm 3.$ $\Delta K = \pm 1, \Delta l_4 = \mp 2.$
			Diagonal Terms. $\Delta K = \pm 6.$ $\Delta K = \pm 2, \Delta l_4 = \pm 2.$ $\Delta K = \pm 4, \Delta l_4 = \mp 2.$

Note : for the non-diagonal elements only the quantum numbers which are varying are indicated.

